

Supporting Information

POM-FLPs: $[\text{Mo}^{\text{IV}}_3]_n$ -Polyoxometalate Bifunctional Catalysis by $[\text{Mo}^{\text{IV}}_3]_n\text{-O}_m$ Lewis Pairs Frustrated by Triangular $\text{Mo}^{\text{IV}}\text{-Mo}^{\text{IV}}$ Bonds

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Contents

1. Figures-XPS

Figure S1. XPS of **1** and **2**. S2

2. Figures-IR

Figure S2. IR of **1** and **2**. S3

3. Figures-TGA

Figure S3. TGA of **1** and **2**. S4

4. Figures-MOs

Figure S4. MOs of **1**. S4

Figure S5. MOs of **2b**. S5

Figure S6. MOs of **3**. S6

Figure S7. MOs of **4**. S7

Figure S8. MOs of **5**. S8

Figure S9. MOs of **6**. S9

5. Tables-BVS

Table S1. Bond valance sum analyses for **1**. S9

Table S2. Bond valance sum analyses for **2**. S10

6. Table-Muliken charge

Table S3. Muliken charge of Mo^{IV} and O for **1-7**. S12

7. Selected bond length data

Table S4. Selected bond length of the DFT-Optimized Structures and crystal structures for **1-7**. S12

8. Cartesian coordinates in xyz file format, in units of Angstrom

B3LYP-6-31G* (C, H, O, N)/LanL2DZ (Mo)-optimized geometry of **1**. S13

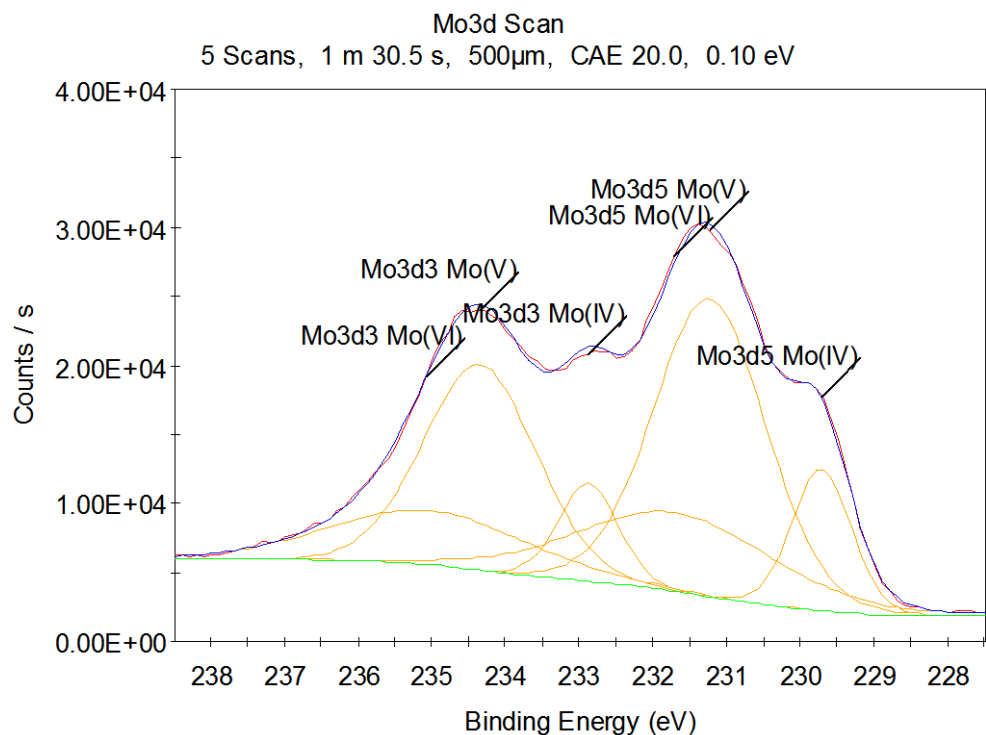
B3LYP-6-31G* (C, H, O, N)/LanL2DZ (Mo, Ge)-optimized geometry of **2b**. S14

B3LYP-6-31G* (C, H, O, N)/LanL2DZ (Mo)-optimized geometry of **3**. S16

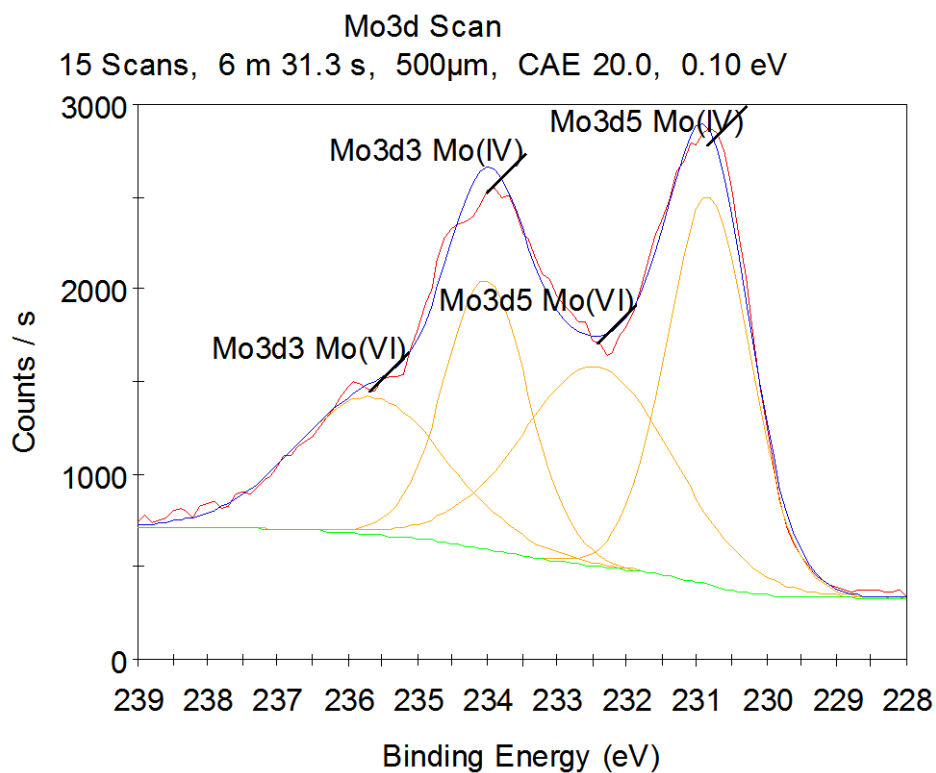
B3LYP-6-31G* (C, H, O, N)/LanL2DZ (Mo)-optimized geometry of **4**. S17

B3LYP-6-31G* (C, H, O, N, Na)/LanL2DZ (Mo)-optimized geometry of **5**. S19

B3LYP-6-31G* (C, H, O, N, P)/LanL2DZ (Mo, Zn)-optimized geometry of **6**. S21

9. The proposed catalytic cycle reported in our previous work**10. References****1. Figures-XPS**

xps of compound 1, C1s: 284.09ev



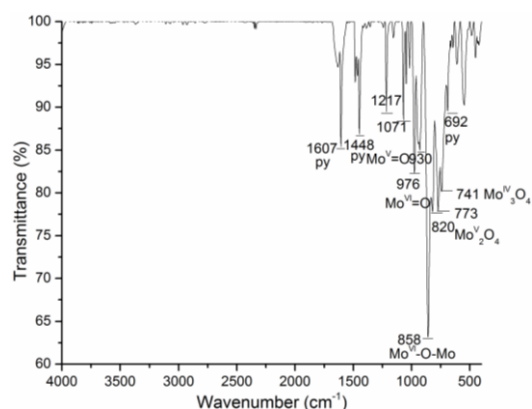
xps of compound **2**, C1s:283.98ev

Binding energies of Mo 3d from the literatures²²⁻²⁷ and the binding energies of peaks used to assign species from the present measurements of **1** and **2** (C1S calibrated to 284.5ev for contrast).

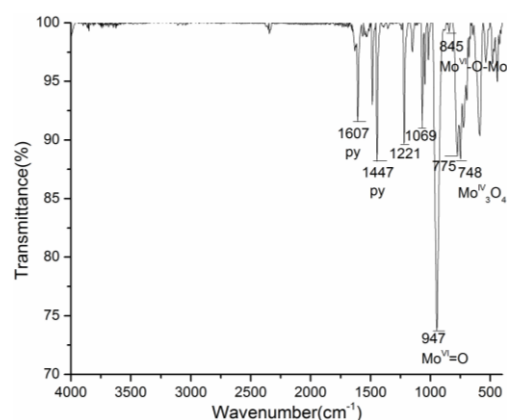
Oxidation state	Mo 3d _{5/2} (eV)	Mo 3d _{3/2} (eV)
Mo(IV)-MoO(OH) ₂	230.2	233.4
Mo(V)-MoCl ₅	230.9-231.1	234.3-235.4
Mo(VI)-Na ₂ MoO ₄ 2H ₂ O	231.9-232.3	235-235.4
Mo(IV) - 1	230.11	233.27
Mo(V) - 1	231.63	234.74
Mo(VI) - 1	232.11	235.46
Mo(IV) - 2	231.35	234.53
Mo(VI) - 2	232.95	236.18
MoIV- γ - 3	229.90	233.13
MoVI- γ - 3	231.81	234.94
MoIV- β - 4	230.0	233.2
MoVI- β - 4	231.9	235.05
Mo(IV) - 5	229.12	232.28
Mo(V) - 5	230.26	233.30
Mo(VI) - 5	231.14	234.20
Mo(IV) - 6	230.0	233.2
Mo(VI) - 6	231.9	235.05

Figure S1. XPS of **1- 6**.

2. Figures-IR



IR of **1**.



IR of **2**

Figure S2. IR of **1** and **2**.

3. Figures-TGA

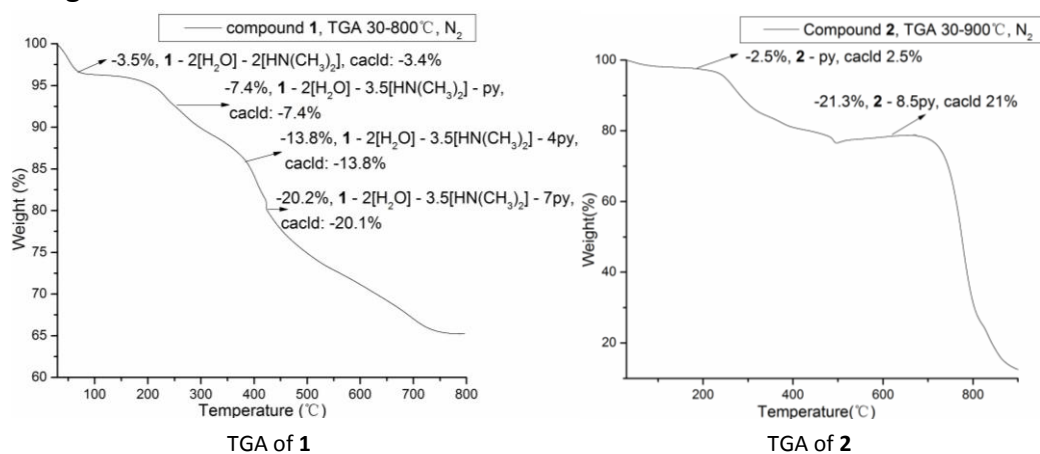


Figure S3. TGA of **1** and **2**.

4. Figures-MOs

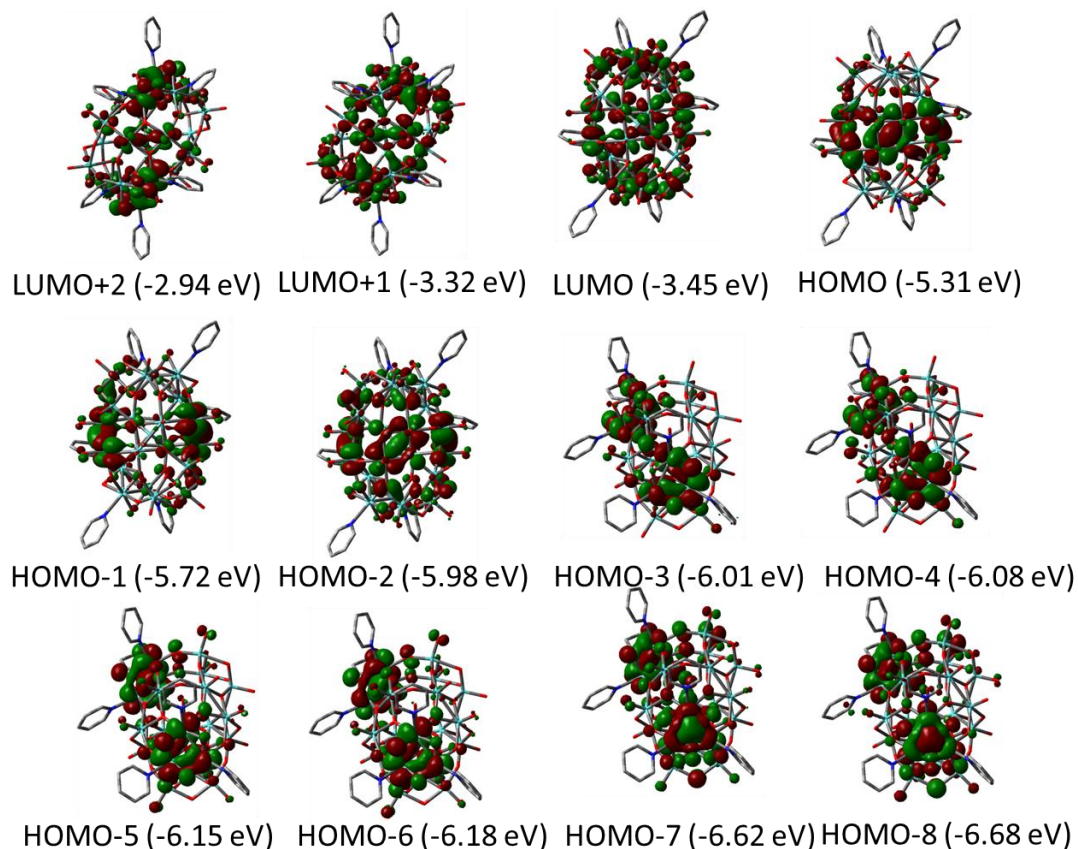


Figure S4. MOs of **1**.

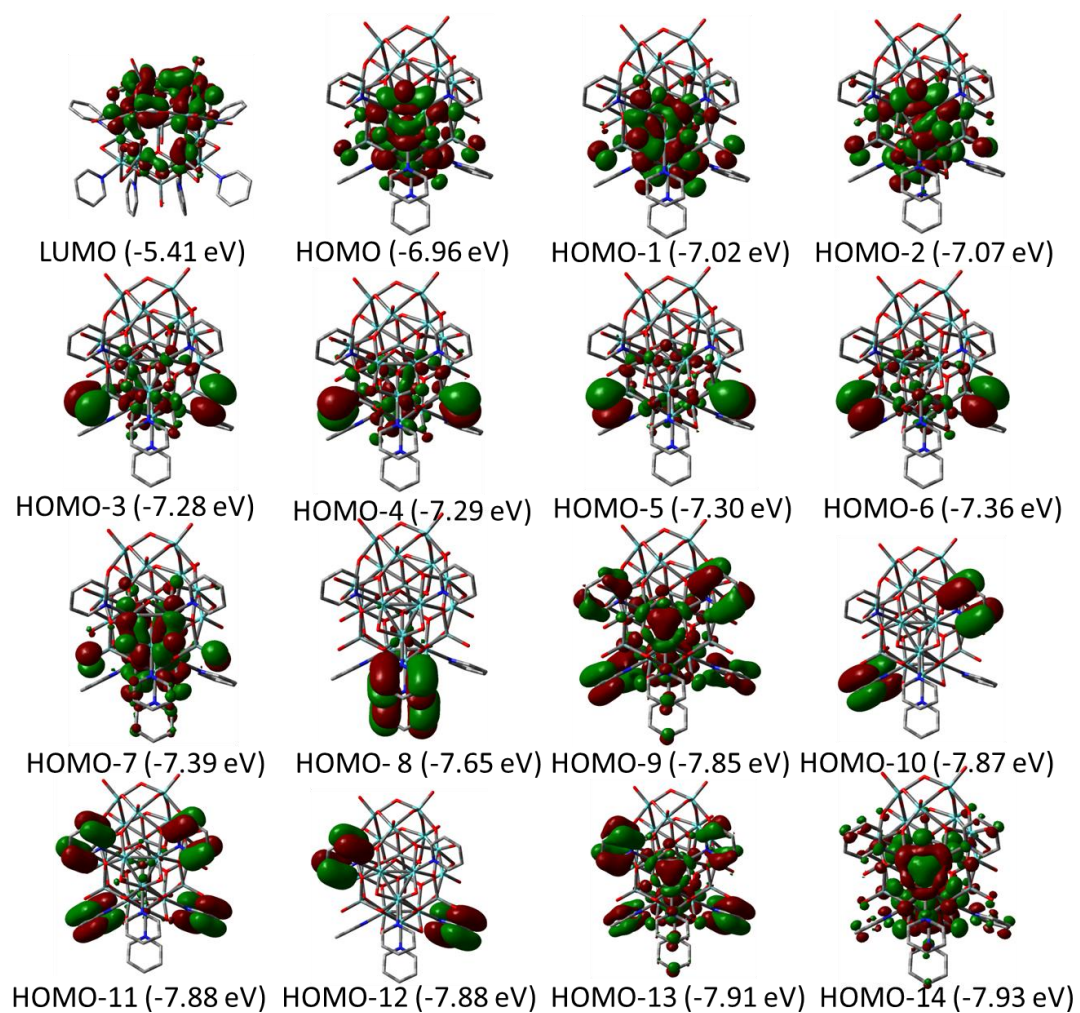


Figure S5. MOs of **2b**.

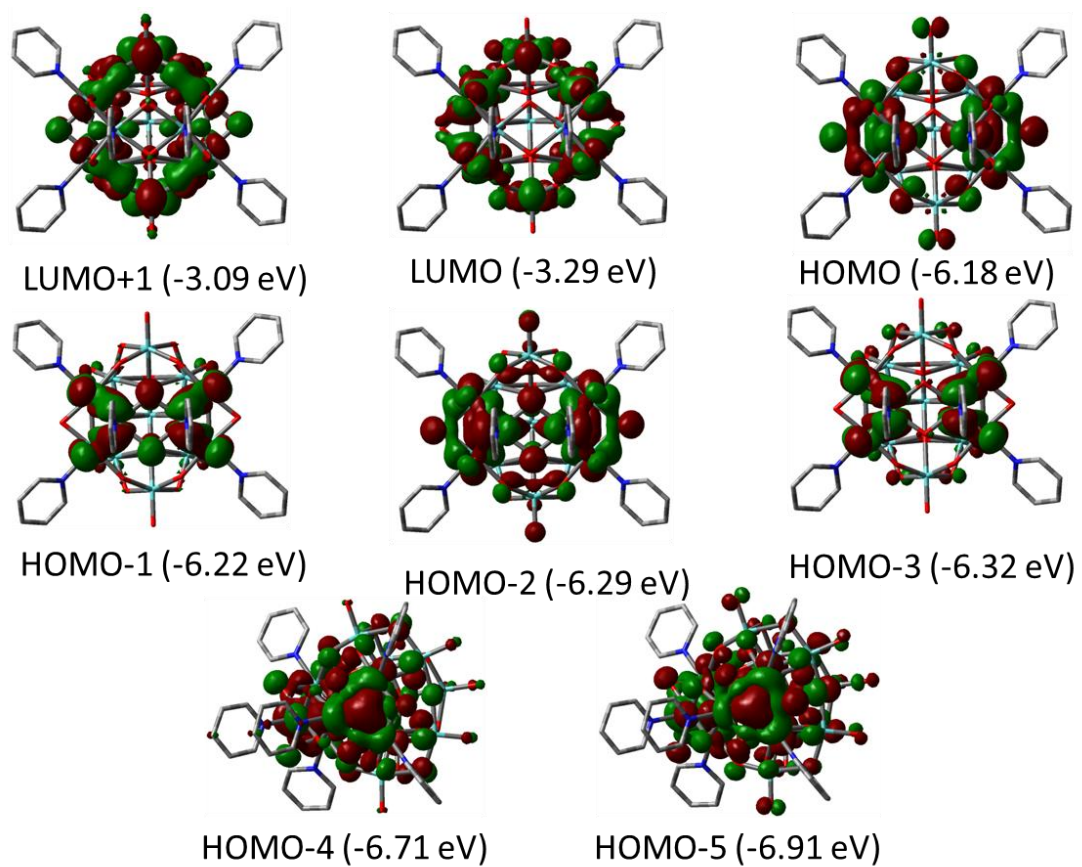


Figure S6. MOs of **3**.

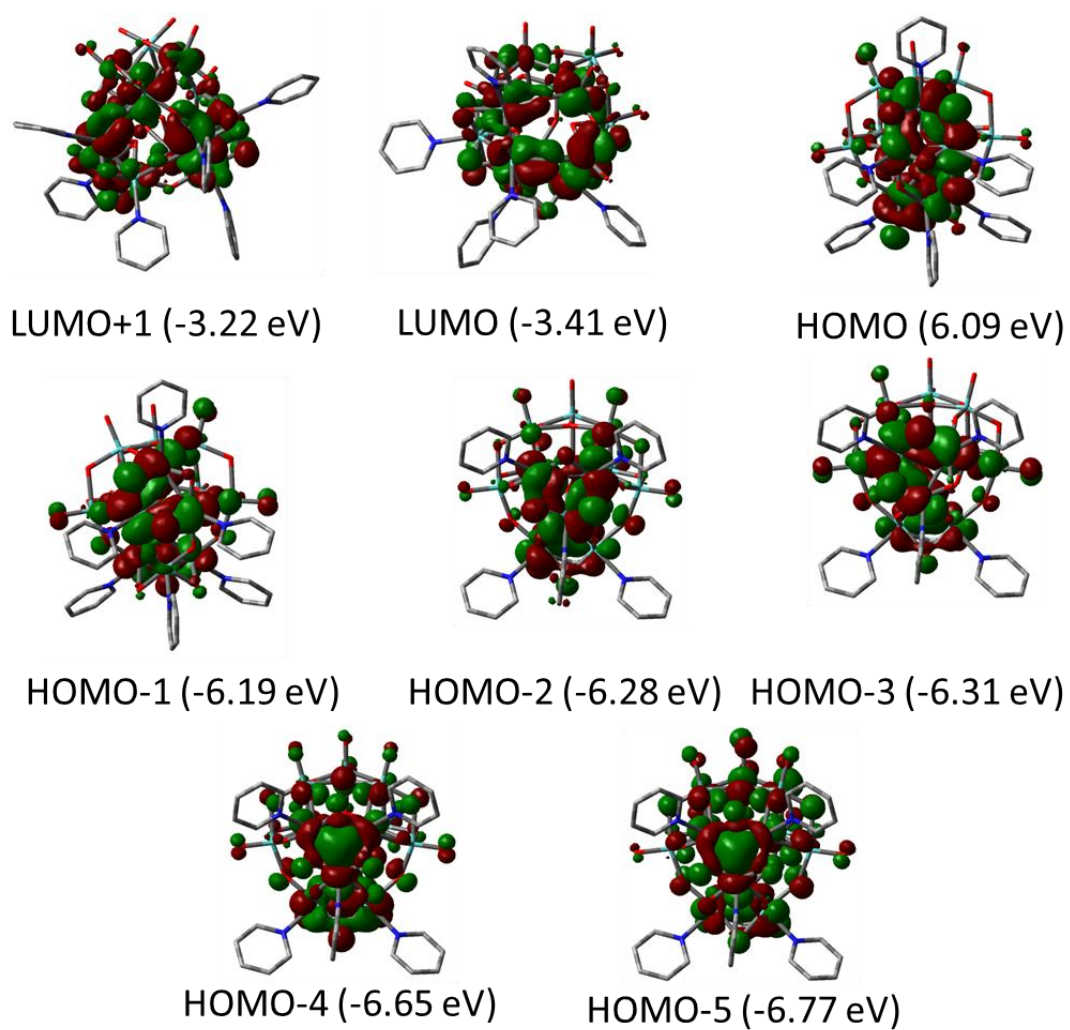


Figure S7. MOs of **4**.

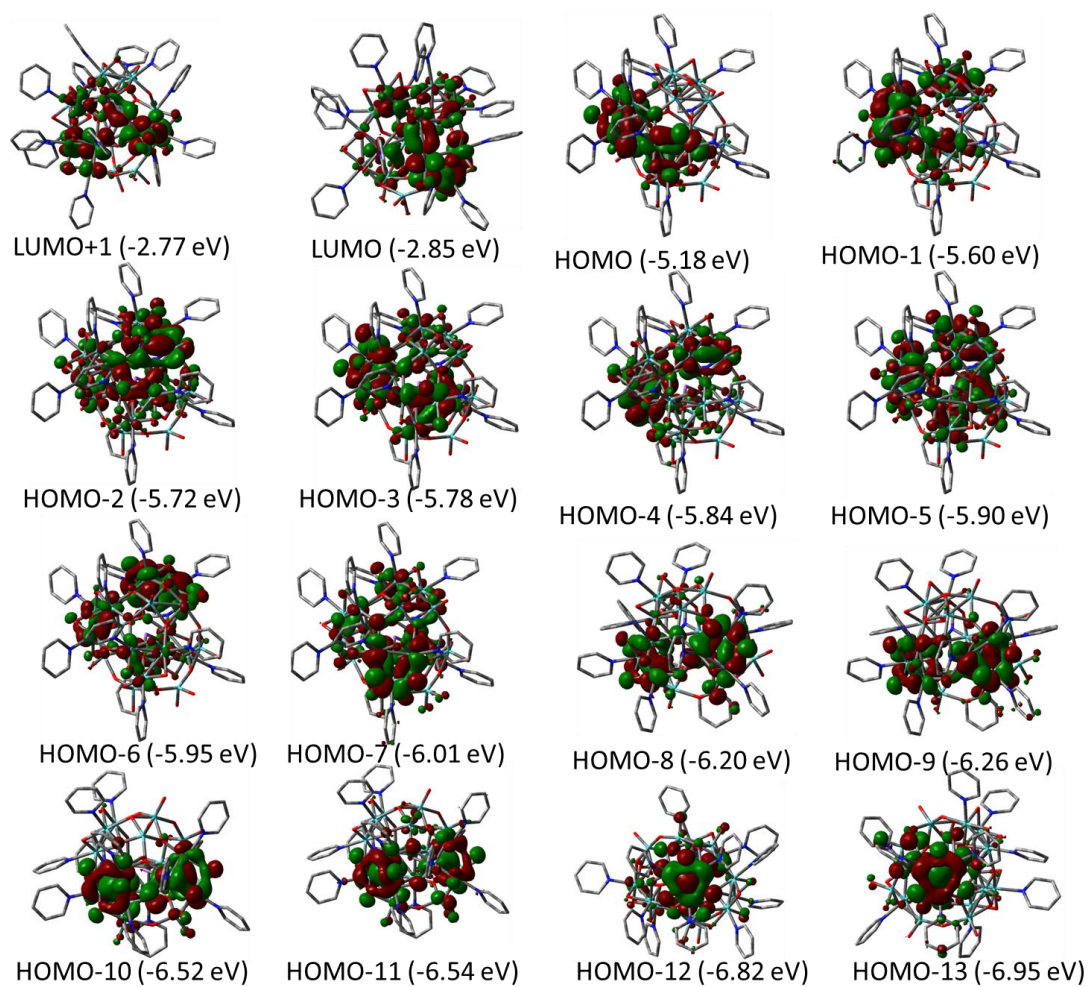


Figure S8. MOs of **5**.

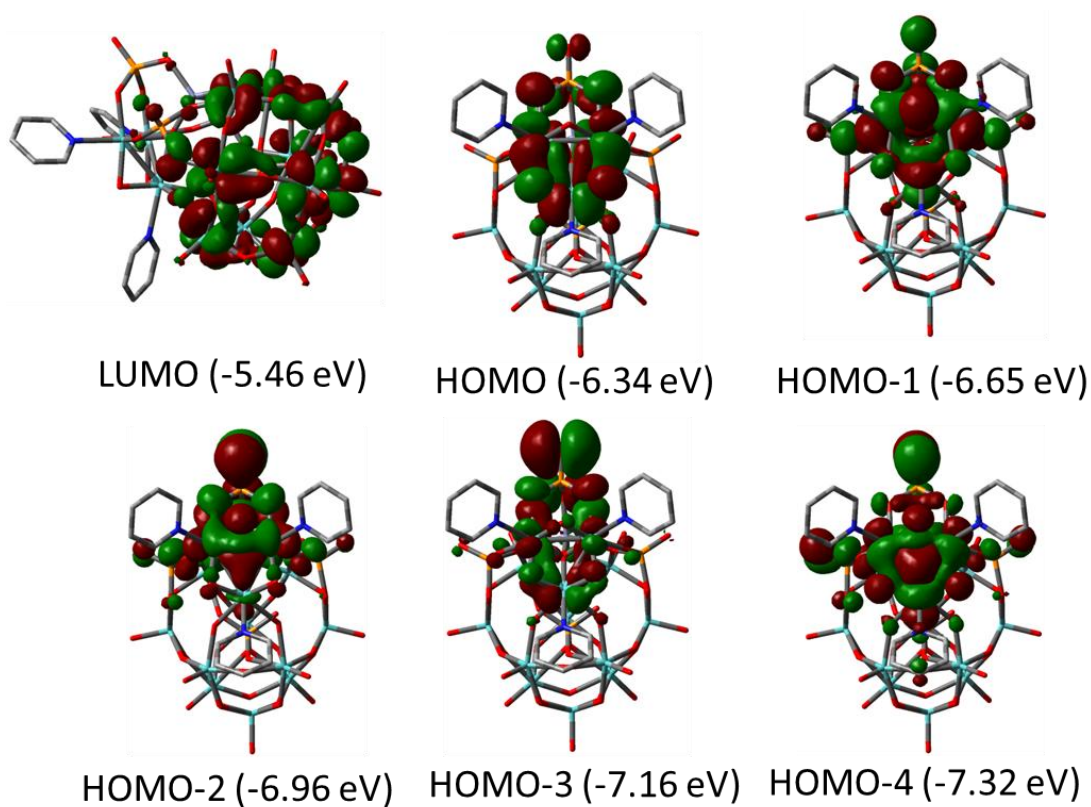


Figure S9. MOs of **6**.

5. Tables-BVS

Table S1. Bond valence sum analyses for **1**.

Atom	Coord	D_aver	Sigm	Distort($\times 10^{-4}$)	Valence	BVSum(Sigma)
Mo1	6.00	2.0625(25)		29.121	4.000	4.113(29)
O1	2.00	1.9290(42)		0.090	-2.000	1.781(20)
Mo2	6.00	2.0562(23)		29.055	4.000	4.156(27)
O2	2.00	1.9268(42)		0.584	-2.000	1.793(20)
Mo3	6.00	2.0395(25)		20.709	4.000	4.301(29)
O3	2.00	1.9415(39)		0.001	-2.000	1.722(18)
Mo4	4.00	1.7601(23)		0.100	6.000	5.950(37)
O4	3.00	2.0290(31)		0.091	-2.000	2.038(17)
Mo5	6.00	1.9728(23)		139.807	6.000	5.955(42)
O5	2.00	2.0992(41)		4.527	-2.000	1.169(13)
Mo7	6.00	2.0098(23)		121.684	5.000	5.346(41)
O7	2.00	1.9364(38)		43.297	-2.000	1.922(21)

Mo10	6.00	1.9681(22)	124.169	6.000	5.995(43)
O10	2.00	1.9529(37)	24.513	-2.000	1.827(19)
O17	3.00	2.2396(30)	2.064	-2.000	1.226(10)
O16	2.00	1.9134(37)	17.241	-2.000	2.011(21)
Mo9	6.00	2.0136(20)	93.125	5.000	5.163(35)
O9	1.00	1.6961(63)	0.000	-2.000	1.768(30)
O13	1.00	1.6731(65)	0.000	-2.000	1.882(33)
O19	1.00	1.6970(66)	0.000	-2.000	1.764(32)
O15	2.00	1.9230(43)	28.146	-2.000	1.989(24)
Mo8	6.00	1.9563(23)	111.767	6.000	6.060(45)
O8	3.00	2.0882(33)	3.717	-2.000	1.820(17)
O18	2.00	1.9143(38)	34.029	-2.000	2.011(21)
Mo11	6.00	1.9509(23)	91.340	6.000	6.005(43)
O11	2.00	1.9515(38)	1.076	-2.000	1.776(18)
O14	1.00	1.6735(65)	0.000	-2.000	1.880(33)
Mo6	6.00	2.0045(23)	86.889	5.000	5.249(40)
O6	3.00	2.0446(31)	9.709	-2.000	2.068(18)
O24	1.00	1.6786(57)	0.000	-2.000	1.854(29)
O23	2.00	1.9798(39)	74.456	-2.000	1.821(21)
O22	2.00	2.0043(38)	135.664	-2.000	1.854(21)
O21	3.00	2.0578(29)	7.787	-2.000	2.019(16)
O20	2.00	1.9727(42)	0.022	-2.000	1.675(19)
O26	1.00	1.6946(62)	0.000	-2.000	1.775(30)
O25	2.00	1.9376(43)	63.702	-2.000	1.971(24)
O29	1.00	1.6930(57)	0.000	-2.000	1.783(28)
O28	3.00	2.1606(26)	169.190	-2.000	2.059(19)
O27	3.00	2.0338(31)	7.264	-2.000	2.152(18)
N3	1.00	2.2107(77)	0.000	-3.000	0.636(13)
N1	1.00	2.2160(89)	0.000	-3.000	0.627(15)
O12	3.00	2.1755(26)	189.374	-2.000	2.061(19)
N2	1.00	2.2408(59)	0.000	-3.000	0.586(9)

Table S2. Bond valence sum analyses for **2**.

Atom	Coord	D_aver	Sigm	Distort(x10 ⁻⁴)	Valence	BVSum(Sigma)
Mo1	6.00	2.0544(35)		30.735	4.000	4.194(41)
N1	1.00	2.2324(126)		0.000	-3.000	0.599(20)
O1	2.00	1.9313(54)		0.416	-2.000	1.770(26)
Ge1	4.00	1.7500(39)		0.273	4.000	3.979(42)
Mo2	6.00	2.0530(32)		28.611	4.000	4.177(36)
Ge2	4.00	1.7908(43)		3.034	4.000	3.576(44)
Zn1	4.00	1.7908(43)		3.034	2.000	3.175(39)
O2	2.00	1.9310(54)		0.000	-2.000	1.771(26)

Mo3	6.00	2.0545(32)	32.933	4.000	4.206(36)
N3	1.00	2.2332(107)	0.000	-3.000	0.598(17)
O3	3.00	2.0104(42)	0.102	-2.000	2.144(24)
Mo4	6.00	2.0510(26)	26.938	4.000	4.200(30)
O4	3.00	1.9653(32)	63.373	-2.000	1.882(17)
Mo5	6.00	1.9736(29)	89.020	6.000	5.674(53)
O5	2.00	1.9320(48)	0.982	-2.000	1.769(23)
Mo6	6.00	1.9827(28)	125.686	6.000	5.796(56)
O6	2.00	1.9174(39)	0.000	-2.000	1.837(19)
Mo7	6.00	1.9660(27)	90.980	6.000	5.752(47)
O7	3.00	2.0130(45)	0.032	-2.000	2.128(26)
O17	1.00	1.6885(105)	0.000	-2.000	1.805(51)
O13	2.00	1.8917(60)	3.201	-2.000	2.093(34)
O18	2.00	1.9260(41)	0.000	-2.000	1.900(21)
O14	2.00	1.9381(58)	45.659	-2.000	1.955(36)
O12	1.00	1.6889(103)	0.000	-2.000	1.803(50)
O11	3.00	2.0822(46)	3.295	-2.000	1.844(23)
O8	3.00	1.9558(42)	57.133	-2.000	1.969(23)
Mo8	6.00	1.9744(33)	88.656	6.000	5.654(63)
O9	3.00	1.9540(30)	54.667	-2.000	1.982(18)
Mo9	6.00	1.9782(36)	125.299	6.000	5.850(68)
Mo10	6.00	1.9693(32)	94.913	6.000	5.732(63)
O10	1.00	1.7368(84)	0.000	-2.000	1.002(26)
O19	2.00	1.8866(51)	0.008	-2.000	2.113(29)
O26	2.00	1.9307(33)	0.000	-2.000	1.876(17)
O25	4.00	2.1707(36)	119.732	-2.000	1.985(22)
O24	2.00	1.9443(47)	41.164	-2.000	1.912(27)
O23	1.00	1.6817(84)	0.000	-2.000	1.839(42)
O22	3.00	2.0828(31)	4.604	-2.000	1.846(16)
N4	1.00	2.2372(78)	0.000	-3.000	0.592(12)
N2	1.00	2.2535(111)	0.000	-3.000	0.566(17)
O20	1.00	1.6944(67)	0.000	-2.000	1.777(32)
O21	2.00	1.8844(55)	1.928	-2.000	2.131(32)
O29	3.00	2.0910(37)	140.151	-2.000	1.777(21)
O28	2.00	1.9027(51)	0.279	-2.000	2.024(28)
O27	1.00	1.6798(80)	0.000	-2.000	1.848(40)
O15	1.00	1.6915(90)	0.000	-2.000	1.790(43)
O16	4.00	2.1759(39)	122.384	-2.000	1.967(27)

6. Table Mulliken charge

Table S3. Mulliken charge of Mo^{IV} and O for **1-7**.

Cluster	Mulliken charge		Mulliken charge mean (O)			
	(Mo ^{IV})					
	mean	Δ	μ_2 -O			Mo=O $\times$ m
			Mo ^{IV} -O-M	Mo ^V -O-Mo ^{V,VI}	Mo ^{VI} -O-Mo ^{VI}	
			$\times$ m	$\times$ m	$\times$ m	
Mo ^{IV} ₆ Mo ^V ₆ Mo ^{VI} ₉	1.407	0.190	-0.785	-0.775	-0.713	-0.550
1			$\times$ 6	$\times$ 8	$\times$ 6	$\times$ 14
Ge ₃ Mo ^{IV} ₆ Mo ^{VI} ₁₀	1.472	0.255	no	no	-0.714	-0.458 $\times$ 10,
2b					$\times$ 14	(Ge=O, -0.840 $\times$ 2)
Mo ^{IV} ₆ Mo ^{VI} _{7-γ}	1.367	0.150	-0.772	no	-0.723	-0.556
3			$\times$ 8		$\times$ 4	$\times$ 8
Mo ^{IV} ₆ Mo ^{VI} _{7-β}	1.368	0.151	-0.771	no	-0.722	-0.561
4			$\times$ 8		$\times$ 4	$\times$ 8
NaMo ^{IV} ₁₂ Mo ^V ₄ Mo ^{VI} ₃	1.395	0.161	-0.807	-0.778	no	-0.556
5			$\times$ 5	$\times$ 2		$\times$ 8
P ₄ Mo ^{IV} ₃ Mo ^{VI} ₁₀ Zn	1.312	0.095	-0.726	no	-0.746	-0.457 $\times$ 10,
6			$\times$ 4		$\times$ 18	(P=O, -0.622 $\times$ 3)
[Mo ₃ O ₄ (C ₂ O ₄) ₃ (py-CH ₃) ₃] ²⁻	1.217	0	no	no	no	no
7						

7. Selected bond length data.

Table S4. Selected bond length of the DFT-Optimized Structures and crystal structures for **1-7**.

Cluster	d(Mo-Mo)		d(Mo-O)			
	Mo ^{IV} -Mo ^{IV}	Mo ^V -Mo ^V	Mo ^{IV} -(μ_2 -O)- Mo ^{IV}	Mo ^{IV} -(μ_3 -O)- Mo ^{IV}	Mo ^{IV} -(μ_2 -O)-Mo ^V VI	Mo ^{IV} -(μ_3 -O)-Mo ^V VI
Mo ^{IV} ₆ Mo ^V ₆ Mo ^{VI} ₉ 1	2.542-2.565	2.731-2.747	1.919-1.978	2.037-2.064	2.060-2.072	2.146-2.209
crystal structure 1	2.497-2.519	2.710-2.734	1.914-1.945	2.024-2.039	2.028-2.094	2.134-2.144
Ge ₃ Mo ^{IV} ₆ Mo ^{VI} ₁₀ 2b	2.508-2.524		1.909-1.968	2.022-2.046		2.098-2.252
crystal structure 2b	2.459-2.499		1.914-1.952	2.007-2.019		2.084-2.100
Mo ^{IV} ₆ Mo ^{VI} _{7-γ} 3	2.554-2.556		1.928-1.962	2.044-2.076	2.039-2.166	
crystal structure 3	2.508-2.517		1.910-1.934	2.016-2.049	2.052-2.129	
Mo ^{IV} ₆ Mo ^{VI} _{7-β} 4	2.549-2.567		1.934-1.970	2.047-2.058	2.038-2.163	
crystal structure 4	2.513-2.532		1.924-1.952	2.023-2.036	2.061-2.120	
NaMo ^{IV} ₁₂ Mo ^V ₄ Mo ^{VI} ₃ 5	2.535-2.597	2.702-2.706	1.876-2.046	2.060-2.082	1.973-2.069	2.070-2.234
crystal structure 5	2.484-2.564	2.670-2.679	1.875-1.994	2.031-2.073	1.936-2.055	2.074-2.190
P ₄ Mo ^{IV} ₃ Mo ^{VI} ₁₀ Zn 6	2.521-2.589		1.895-1.990			2.228-2.261
crystal structure 6	2.517-2.563		1.922-1.961			2.137
[Mo ₃ O ₄ (C ₂ O ₄) ₃ (py-CH ₃) ₃] ²⁻ 7	2.550-2.552		1.945-1.946	2.074-2.075		
crystal structure 7	2.494-2.506		1.901-1.928	2.033-2.042		

8. Cartesian coordinates in xyz file format, in units of Angstrom

B3LYP-6-31G* (C, H, O, N)/LanL2DZ (Mo)-optimized geometry of 1.

Total electronic charge: -4.

Mo	2.86455265	-1.95037139	1.60317451	N	5.51949826	-3.51936568	-1.56806950
O	4.31843498	-1.30003166	2.76036333	N	2.54579018	-3.44926315	3.25356767
Mo	4.68969276	-0.18667781	1.23556898	C	5.22731384	-4.82968299	-1.45559431
O	3.91554397	-3.35631582	0.82877111	H	4.37521677	-5.07329886	-0.83254536
Mo	4.25284598	-1.96048119	-0.53168428	C	6.57456355	-3.14917775	-2.31945533
O	5.92565889	-1.35936929	0.32244919	H	6.76098243	-2.08393938	-2.38665827
Mo	-0.00000812	0.36406189	-0.00002022	C	2.64792063	-3.07298240	4.54284800
O	2.99795840	-0.50294230	0.13843471	H	2.86077174	-2.02586197	4.71694691
Mo	-0.83606913	-3.01319352	1.41663376	C	2.29096923	-4.74062920	2.97105406
O	3.59263636	1.38243494	2.25661381	H	2.21762341	-4.99365412	1.92109327
Mo	1.72385754	1.43585890	3.16623245	C	5.97767807	-5.81410271	-2.09142375
O	5.12182896	1.45385684	0.04648051	H	5.70433548	-6.85703027	-1.97320768
Mo	1.78045594	3.11717893	-3.13093994	C	7.07225295	-5.43224264	-2.86789647
O	3.14232342	3.36328381	0.20253613	H	7.67778011	-6.17761542	-3.37414631
O	-2.74065942	1.49433285	1.77683183	C	7.37488392	-4.07476159	-2.98206934
O	-2.22181622	-0.41058830	3.69232240	H	8.21577355	-3.73028879	-3.57413788
H	3.60839468	2.18756953	1.69181360	C	2.22327225	-5.30987517	5.30231460
Mo	1.19596924	3.82928154	0.67496271	H	2.09727880	-6.03502199	6.10041687
O	5.62042575	4.02923961	-0.99759504	C	2.12350459	-5.69940953	3.96601991
O	2.24768570	1.62461322	4.78004707	H	1.92000499	-6.72847671	3.69000737
O	-4.69994632	0.18458366	4.87012735	C	2.49123422	-3.97136640	5.59344078
O	-0.33603986	-2.42836620	3.07735741	H	2.58213065	-3.62172340	6.61619397
Mo	-3.85224082	0.40925762	3.38179866	H	-2.36363478	0.90475165	1.10053006
O	1.07929910	-2.66641034	0.65229237	O	1.20160958	1.43469032	0.72599375
O	-2.64811367	-2.78680084	1.52557569	N	6.47355589	0.52453319	2.43580732
Mo	4.43375145	2.77360273	-1.02684075	C	7.57210209	0.99484518	1.81406104
O	1.70483936	3.23554326	2.50594970	H	7.54948584	0.98339137	0.73094939
O	0.07707625	-0.67233649	5.28215094	C	8.67065575	1.48205334	2.51571827
Mo	-0.20330404	-0.44545438	3.61872702	H	9.53401435	1.85028487	1.97233869
O	1.65640532	-0.53368371	2.79120369	C	8.63232035	1.48672666	3.91066882
O	1.38831048	5.51528870	0.83114872	H	9.47291147	1.86308135	4.48540174
O	3.14525993	4.01227498	-2.37514829	C	7.49417460	0.99872980	4.55332718
O	2.70090587	2.12767795	-4.31150617	H	7.41878896	0.98101947	5.63518138
O	0.70284648	3.48914456	-1.25173585	C	6.43737154	0.52447263	3.78249107
O	-4.93975639	1.92747765	2.70534551	H	5.53617507	0.12565768	4.23199067
O	0.94397874	4.28643290	-4.08208712	O	2.64822210	-2.78746024	-1.52434459
O	-4.56415746	-0.84643101	2.24542008	O	4.56427242	-0.84764441	-2.24539479
O	-0.69542186	-4.72426246	1.52396340	O	-0.72282007	-0.59209109	1.32506440
O	0.72290489	-0.59252624	-1.32477839	H	2.36338176	0.90357976	-1.10163709
O	-0.25781362	1.53987233	3.26542877	O	-1.20183096	1.43443103	-0.72612924

O	-1.07909020	-2.66671325	-0.65112860	O	-2.24758238	1.62262084	-4.78060817
O	2.74059500	1.49340139	-1.77761545	O	-4.31838431	-1.30153115	-2.75988797
O	0.25790583	1.53880774	-3.26601449	N	-2.54548559	-3.45072737	-3.25202133
Mo	-1.78070431	3.11866062	3.12949407	N	-6.47372872	0.52282210	-2.43657978
Mo	-4.43413015	2.77357251	1.02559614	C	-5.22691263	-4.82868514	1.45868926
Mo	-1.19611109	3.82895601	-0.67625039	C	-6.57509056	-3.14767063	2.32009916
O	-0.70306439	3.48964523	1.25058689	C	-2.64762789	-3.07515606	-4.54150542
O	-2.70111013	2.12911774	4.31026618	C	-2.29064435	-4.74193831	-2.96880256
Mo	0.83616493	-3.01369389	-1.41542341	C	-7.57196693	0.99451180	-1.81531970
Mo	-4.25264228	-1.96023209	0.53250302	C	-6.43772138	0.52098160	-3.78327452
O	4.93962955	1.92652764	-2.70629526	H	-4.37441318	-5.07270788	0.83636026
Mo	3.85248419	0.40797463	-3.38183797	C	-5.97729749	-5.81265938	2.09518836
Mo	0.20351538	-0.44677468	-3.61853307	H	-6.76187293	-2.08242312	2.38605779
Mo	-1.72384047	1.43460084	-3.16669156	C	-7.37544003	-4.07278579	2.98331996
Mo	-2.86443670	-1.95097647	-1.60242988	H	-2.86046813	-2.02812914	-4.71619199
O	-3.14534984	4.01374850	2.37384285	C	-2.49097262	-3.97411791	-5.59160898
O	-0.94403241	4.28782328	4.08059859	H	-2.21726624	-4.99437640	-1.91870520
O	-5.12243872	1.45390697	-0.04758988	C	-2.12320311	-5.70126360	-3.96324497
O	-3.14251683	3.36303864	-0.20372108	H	-7.54924163	0.98440874	-0.73219836
O	-5.62049798	4.02950278	0.99620848	C	-8.67032342	1.48143102	-2.51747991
O	-1.70494588	3.23443575	-2.50704152	C	-7.49436552	0.99479956	-4.55459533
O	-1.38855021	5.51489240	-0.83314240	H	-5.53680918	0.12105997	-4.23234763
O	0.33619468	-2.42944160	-3.07637153	H	-5.70357960	-6.85562620	1.97820739
O	0.69548841	-4.72479881	-1.52217114	C	-7.07235175	-5.43030115	2.87073519
Mo	-4.68983539	-0.18740638	-1.23567032	H	-8.21670644	-3.72793396	3.57463134
O	-3.91524796	-3.35669966	-0.82725469	C	-2.22301565	-5.31246771	-5.29975158
O	-5.92559570	-1.35968548	-0.32191800	H	-2.58188809	-3.62503652	-6.61455183
O	-2.99798859	-0.50285860	-0.13839531	H	-1.91969004	-6.73017775	-3.68667144
N	-5.51955536	-3.51833857	1.56961399	H	-9.53340728	1.85085444	-1.97447460
O	2.22185777	-0.41187531	-3.69212081	C	-8.63215297	1.48428332	-3.91244065
O	4.69987515	0.18290995	-4.87029487	H	-7.41913785	0.97557766	-5.63643558
O	-0.07707434	-0.67431973	-5.28182376	H	-7.67790229	-6.17531006	3.37749177
O	-1.65628307	-0.53474351	-2.79086367	H	-2.09705637	-6.03805788	-6.09745633
O	-3.59269029	1.38138177	-2.25723574	H	-9.47260026	1.86036456	-4.48756174
H	-3.60855842	2.18675239	-1.69279940				

B3LYP-6-31G* (C, H, O, N)/LanL2DZ (Mo, Ge)-optimized geometry of **2b**.

Total electronic charge: 0.

Mo	3.21116809	-1.64885801	-0.00934541	Ge	2.21028585	0.02704452	-2.88520177
N	5.44816897	-1.70256382	0.00750532	O	1.32269839	-4.45780263	0.02076023
O	3.39034837	-2.91117691	-1.50284186	Mo	3.21109710	1.64902113	0.00951299
Ge	-1.71125608	-0.00002183	-0.00000656	N	5.44808383	1.70284251	-0.00724298
Mo	1.49588804	-3.00474184	-1.24278600	O	1.17574602	-1.44177601	0.00054421

Mo	1.51440039	2.96995283	-1.28108383	H	9.28335309	-2.20294807	0.15207058
O	3.19456187	0.00356669	-1.33634852	C	0.78912413	5.61753707	-2.80796581
Mo	-0.99944281	1.76333653	-2.95708562	H	0.22752571	5.74196263	-1.88971586
O	3.41012383	2.90403353	-1.49365640	C	2.09314692	-4.25598172	-4.05349763
Mo	-1.98570242	3.62871381	0.24200234	H	2.53367788	-3.27095444	-4.15509820
O	1.32247594	4.45787343	-0.02084001	C	0.94162052	-5.74839398	-2.68856355
Mo	-4.36228280	2.13041492	-1.58226540	H	0.50214122	-5.93213173	-1.71550837
O	1.17567262	1.44185009	-0.00059192	C	0.92577069	-6.71146975	-3.69085982
O	-5.45889296	-2.36227516	-2.81619590	H	0.45493060	-7.67009105	-3.50342911
O	-2.75189748	-1.63197253	-2.86851787	C	2.11970217	-5.17158286	-5.09868841
O	-5.24169455	-2.12497975	-0.05605788	H	2.59785765	-4.90168170	-6.03364063
O	-3.38801977	-3.64906271	-1.34220568	C	2.25986453	4.28908673	-4.02778703
O	-0.75533490	-2.74988258	-4.36389849	H	2.83847671	3.37389582	-4.06616257
O	-0.69386851	-2.90712499	-1.44173264	C	1.52460406	-6.42093371	-4.91741592
O	1.09992417	-1.48357939	-2.71344582	H	1.52882755	-7.15500670	-5.71687677
Mo	-0.85605733	-1.54161649	-3.16822517	C	0.74779721	6.56821062	-3.82136644
O	1.12704831	1.49130871	-2.71825707	H	0.13651604	7.45518958	-3.69749563
Mo	-1.98540121	-3.62877845	-0.24199389	C	1.50068204	6.35719632	-4.97744764
Mo	-4.29622325	-1.69140124	-1.77293471	H	1.48822857	7.08348924	-5.78391305
O	3.09387610	-0.03589156	-4.27905376	O	-1.52650675	-5.25563931	-0.06944090
O	-4.64265087	0.07732219	-1.74535192	C	2.27080768	5.19763960	-5.07919329
O	-5.24183613	2.12472918	0.05603613	H	2.87224819	4.99201298	-5.95759992
O	-2.76078745	1.44623494	0.05390135	O	-2.76073266	-1.44631726	-0.05394832
O	-3.38831301	3.64884665	1.34224517	O	3.41017552	-2.90390365	1.49372959
O	-1.52690255	5.25560301	0.06948444	Mo	1.51441547	-2.96991558	1.28103137
O	-0.72687271	2.93148902	-1.49520778	O	3.19451220	-0.00343551	1.33642592
N	1.53083990	4.49425919	-2.91092023	C	6.11180503	-1.58373897	1.17671845
N	1.51228057	-4.53794402	-2.86789548	O	-0.94645202	-0.03937059	1.55928838
O	-5.54416988	2.62160384	-2.69507477	Mo	1.49563439	3.00485500	1.24273530
O	-2.80069173	1.66925123	-2.87539631	O	3.39013723	2.91136142	1.50290796
C	6.14479029	-1.99130863	-1.11200457	C	6.14464191	1.99164492	1.11229336
H	5.56955885	-2.08600992	-2.02440165	O	-3.36018812	3.62769383	-1.30124843
O	-0.94647732	0.03941728	-1.55935468	O	-0.69405150	2.90724125	1.44172541
O	-0.77691632	-0.00036198	-4.09778017	Mo	-4.36216297	-2.13067381	1.58220094
O	-0.75626129	2.72857011	-4.34297025	O	-3.35996279	-3.62787000	1.30125885
C	8.20819341	2.06006933	-0.11039136	O	-0.72665632	-2.93152598	1.49520709
H	9.28323964	2.20348898	-0.15165978	Mo	-4.29643672	1.69122237	1.77285102
C	7.52248119	-2.17525878	-1.09870164	C	7.52231979	2.17568932	1.09904308
H	8.03919261	-2.40748651	-2.02325273	C	7.48826808	-1.75408430	1.26650836
C	7.48823030	1.75448840	-1.26616341	O	1.12702749	-1.49125967	2.71825683
H	7.97804263	1.64978412	-2.22777840	N	1.53090133	-4.49428135	2.91080462
C	6.11177524	1.58404970	-1.17642774	Ge	2.21014853	-0.02690736	2.88527738
H	5.51379367	1.34892197	-2.04846177	H	5.51377266	-1.34866377	2.04873171
C	8.20829845	-2.05960352	0.11076112	Mo	-0.85625985	1.54154411	3.16812059

Mo	-0.99931621	-1.76339518	2.95721244	C	2.09275589	4.25620077	4.05344011
O	1.09980751	1.48362694	2.71337769	H	2.83989597	-3.37483011	4.06537786
N	1.51191584	4.53809260	2.86781036	C	2.27157647	-5.19824505	5.07864505
H	5.56936951	2.08631544	2.02466716	H	0.22623701	-5.74111435	1.89023911
O	-5.54405647	-2.62187445	2.69500620	C	0.74704422	-6.56779437	3.82155016
O	-2.80054013	-1.66930821	2.87530305	H	0.50169942	5.93217168	1.71535907
O	-4.64260408	-0.07752314	1.74527808	C	0.92516555	6.71157452	3.69072047
O	-5.45907897	2.36190237	2.81626131	H	2.53337857	3.27121784	4.15506929
O	-2.75199140	1.63185358	2.86846709	C	2.11917827	5.17181686	5.09862159
H	8.03897819	2.40796205	2.02361239	H	2.87361301	-4.99304520	5.95674271
H	7.97803475	-1.64935776	2.22814438	C	1.50066975	-6.35731353	4.97724621
C	2.26065184	-4.28963201	4.02729051	H	0.13514579	-7.45438528	3.69795174
C	0.78842630	-5.61708680	2.80818305	H	0.45424428	7.67014969	3.50325656
O	3.09374876	0.03604689	4.27912137	C	1.52397076	6.42110881	4.91730792
O	-0.77690005	0.00026391	4.09772713	H	2.59731422	4.90196993	6.03359983
O	-0.75545131	2.74980202	4.36380473	H	1.48818682	-7.08364106	5.78368053
O	-0.75625454	-2.72879124	4.34299472	H	1.52809057	7.15519164	5.71675971
C	0.94115067	5.74848807	2.68843722				

B3LYP-6-31G* (C, H, O, N)/LanL2DZ (Mo)-optimized geometry of **3**.

Total electronic charge: -2.

Mo	1.93304789	1.81965901	2.71470785	C	3.98814736	4.33841074	0.01824078
Mo	-0.00000000	1.69749367	-2.56632793	H	4.05076031	3.44351134	0.62603974
Mo	1.27815739	2.89152922	-0.70592894	C	-1.20122162	2.07953018	-6.86893305
Mo	0.00000000	0.00000000	4.77841220	H	-2.15925366	2.13002170	-7.37469897
Mo	3.50488391	-0.00000000	0.36643001	C	4.86449787	6.42402040	-0.78732272
O	-0.00000000	1.30692690	-0.52763603	H	5.63943856	7.18397063	-0.80870730
O	-0.00000000	1.59400063	3.10144270	C	2.74209374	5.56719337	-1.50782421
O	1.55179431	2.94280370	1.31414410	H	1.82926799	5.63190487	-2.08782537
O	1.54977902	-0.00000000	1.37654154	C	0.00000000	2.14742650	-7.57573806
O	1.27768036	-0.00000000	-2.85524569	H	0.00000000	2.25238256	-8.65622159
O	0.00000000	4.36705621	-0.64828035	C	5.00223683	5.29141914	0.01581191
O	1.48602868	2.92209225	-2.65643701	H	5.87974826	5.14028420	0.63509710
O	2.87026928	1.42731092	-0.59951930	C	3.71223726	6.56256662	-1.56209004
O	1.81201928	-0.00000000	3.98378458	H	3.55953074	7.42590840	-2.20052429
O	2.39488190	2.86408965	4.00538346	H	1.98424120	-0.00000000	-2.17860873
O	5.21802150	-0.00000000	0.11869918	H	0.85210670	-0.00000000	0.69919573
O	-0.00000000	1.34575774	5.86439556	Mo	-1.27815739	2.89152922	-0.70592894
O	3.57036081	1.28818494	2.04876319	O	-1.27768036	0.00000000	-2.85524569
N	2.87681900	4.47392694	-0.73203270	O	-1.48602868	2.92209225	-2.65643701
N	-0.00000000	1.87924979	-4.80405199	H	-1.98424120	0.00000000	-2.17860873
C	-1.16067757	1.94611131	-5.48500685	O	-0.00000000	-1.59400063	3.10144270
H	-2.06477159	1.89708922	-4.89086124	O	-1.81201928	0.00000000	3.98378458

O	-0.00000000	-1.34575774	5.86439556	O	-5.21802150	0.00000000	0.11869918
O	2.87026928	-1.42731092	-0.59951930	H	-4.05076031	3.44351134	0.62603974
O	3.57036081	-1.28818494	2.04876319	C	-5.00223683	5.29141914	0.01581191
Mo	-1.93304789	1.81965901	2.71470785	H	-1.82926799	5.63190487	-2.08782537
Mo	1.93304789	-1.81965901	2.71470785	C	-3.71223726	6.56256662	-1.56209004
Mo	-0.00000000	-1.69749367	-2.56632793	C	3.98814736	-4.33841074	0.01824078
C	1.16067757	1.94611131	-5.48500685	C	2.74209374	-5.56719337	-1.50782421
C	1.20122162	2.07953018	-6.86893305	C	-3.98814736	-4.33841074	0.01824078
O	-1.55179431	2.94280370	1.31414410	C	-2.74209374	-5.56719337	-1.50782421
O	-2.87026928	1.42731092	-0.59951930	H	2.06477159	-1.89708922	-4.89086124
N	-2.87681900	4.47392694	-0.73203270	C	1.20122162	-2.07953018	-6.86893305
Mo	-1.93304789	-1.81965901	2.71470785	H	-2.06477159	-1.89708922	-4.89086124
Mo	1.27815739	-2.89152922	-0.70592894	C	-1.20122162	-2.07953018	-6.86893305
O	-1.54977902	0.00000000	1.37654154	C	-4.86449787	6.42402040	-0.78732272
O	-2.39488190	2.86408965	4.00538346	H	-5.87974826	5.14028420	0.63509710
O	-3.57036081	1.28818494	2.04876319	H	-3.55953074	7.42590840	-2.20052429
H	-0.85210670	0.00000000	0.69919573	H	4.05076031	-3.44351134	0.62603974
O	1.55179431	-2.94280370	1.31414410	C	5.00223683	-5.29141914	0.01581191
O	2.39488190	-2.86408965	4.00538346	H	1.82926799	-5.63190487	-2.08782537
Mo	-1.27815739	-2.89152922	-0.70592894	C	3.71223726	-6.56256662	-1.56209004
O	-0.00000000	-1.30692690	-0.52763603	H	-4.05076031	-3.44351134	0.62603974
O	-1.48602868	-2.92209225	-2.65643701	C	-5.00223683	-5.29141914	0.01581191
O	1.48602868	-2.92209225	-2.65643701	H	-1.82926799	-5.63190487	-2.08782537
N	-0.00000000	-1.87924979	-4.80405199	C	-3.71223726	-6.56256662	-1.56209004
H	2.06477159	1.89708922	-4.89086124	H	2.15925366	-2.13002170	-7.37469897
H	2.15925366	2.13002170	-7.37469897	C	-0.00000000	-2.14742650	-7.57573806
Mo	-3.50488391	0.00000000	0.36643001	H	-2.15925366	-2.13002170	-7.37469897
C	-3.98814736	4.33841074	0.01824078	H	-5.63943856	7.18397063	-0.80870730
C	-2.74209374	5.56719337	-1.50782421	C	4.86449787	-6.42402040	-0.78732272
O	-1.55179431	-2.94280370	1.31414410	H	5.87974826	-5.14028420	0.63509710
O	-2.39488190	-2.86408965	4.00538346	H	3.55953074	-7.42590840	-2.20052429
O	-3.57036081	-1.28818494	2.04876319	C	-4.86449787	-6.42402040	-0.78732272
O	-0.00000000	-4.36705621	-0.64828035	H	-5.87974826	-5.14028420	0.63509710
N	2.87681900	-4.47392694	-0.73203270	H	-3.55953074	-7.42590840	-2.20052429
O	-2.87026928	-1.42731092	-0.59951930	H	-0.00000000	-2.25238256	-8.65622159
N	-2.87681900	-4.47392694	-0.73203270	H	5.63943856	-7.18397063	-0.80870730
C	1.16067757	-1.94611131	-5.48500685	H	-5.63943856	-7.18397063	-0.80870730
C	-1.16067757	-1.94611131	-5.48500685				

B3LYP-6-31G* (C, H, O, N)/LanL2DZ (Mo)-optimized geometry of **4**.

Total electronic charge: -2.

Mo	2.89232404	0.82498565	1.22894971	Mo	2.81459061	0.83784259	-1.32232809
Mo	1.48455544	2.57434635	0.00539201	Mo	-2.07367865	1.79558606	1.31993640

Mo	-2.13429214	1.78812540	-1.24672608	O	2.99396157	-3.85809265	-2.45683975
Mo	-3.34175362	-0.03110583	0.07395159	N	4.37221236	0.98235167	-2.94510351
Mo	1.89448869	-2.62784780	-1.95947032	C	5.36892050	0.07815368	-3.01153365
Mo	-0.01821960	-0.34319773	-3.52054375	H	5.37350492	-0.68347012	-2.24122070
Mo	-1.76156519	-2.74722746	-1.88977168	C	6.33126547	0.10808131	-4.01590638
Mo	1.97263745	-2.63902501	1.92256215	H	7.11638326	-0.64004987	-4.02872871
Mo	0.11530720	-0.32293340	3.50414436	C	6.26023602	1.10574993	-4.98899172
Mo	-1.67640679	-2.75335282	1.94130966	H	6.99521374	1.15301440	-5.78652559
Mo	0.21714135	-4.75472204	-0.01165081	C	5.22818978	2.04197495	-4.91812059
O	1.27800408	0.52667805	0.00302362	H	5.13345152	2.83642664	-5.65034098
O	-1.33793978	0.38553371	0.02125058	C	4.30582860	1.94957209	-3.88071356
O	0.00481404	-1.35236568	-1.56146490	H	3.49346849	2.65809161	-3.77400143
O	0.10918662	-1.35235264	1.56740895	N	-5.45697909	-0.79652199	0.11965409
O	-2.66675766	-4.12833876	-2.38936156	C	-6.05424478	-1.08052609	1.29319051
O	1.42916885	-2.02678716	3.56217524	H	-5.47290362	-0.88057063	2.18522088
O	3.08504332	-3.88928848	2.33920870	C	-7.34130423	-1.60413699	1.36148313
O	-1.40133641	-3.16096279	0.02174508	H	-7.78298192	-1.81809606	2.32863426
O	0.11297315	-0.13927143	5.22481942	C	-8.03593383	-1.84282364	0.17498533
O	-2.95399400	-1.55187937	1.42419117	H	-9.04125064	-2.25192422	0.19646799
O	2.96680147	-1.17203562	-1.62203695	C	-7.41595511	-1.54672168	-1.03952073
O	-3.94640477	1.11101072	-1.39622218	H	-7.91717439	-1.71504801	-1.98646312
O	1.27470564	-1.99243381	-3.58656032	C	-6.12672846	-1.02412418	-1.02656531
O	1.54547089	0.62402055	2.90955874	H	-5.60217368	-0.77662267	-1.94145714
O	-1.37013189	0.73301623	-2.86480240	N	-2.62828731	3.33576509	2.90255767
O	-3.01898145	-1.56135977	-1.31668452	C	-2.95426412	4.60101045	2.56465706
O	-2.57978363	-4.12127417	2.47524474	H	-2.90467268	4.83319190	1.50766942
O	2.69622823	2.78957619	-1.48865711	C	-3.33634378	5.54817353	3.50920882
O	1.39976214	0.66369031	-2.93574639	H	-3.58512318	6.55376376	3.18779782
O	-0.15475640	2.68509559	-1.40877178	C	-3.39439314	5.17838074	4.85294185
O	0.15004261	-3.96530843	-1.82248122	H	-3.69197185	5.89524273	5.61190763
O	-1.19272704	-1.99724625	3.55422996	C	-3.06395980	3.86864295	5.20227201
O	-1.27108957	0.73678494	2.90880383	H	-3.09532919	3.53312342	6.23316188
O	3.03881753	-1.19004398	1.51806110	C	-2.68445025	2.97872653	4.20279763
O	1.73261751	-3.00766888	-0.03481708	H	-2.40583079	1.95506266	4.42215907
O	-2.53205805	3.19831998	0.01552209	N	1.42196179	4.82963789	0.02695888
O	-1.34374759	-1.99236641	-3.52832084	C	2.54500922	5.53804978	0.26194144
O	0.22119576	-3.96508345	1.80711130	H	3.43625528	4.96128318	0.47766849
O	2.77890083	2.77498398	1.43114561	C	2.56288282	6.92855069	0.24029889
O	-3.89517281	1.15490216	1.52381725	H	3.49102658	7.45539395	0.43324540
O	4.32293574	0.84728467	-0.08670098	C	1.37803329	7.61543350	-0.02779202
O	-0.13338005	2.70668204	1.33923153	H	1.36126842	8.70061496	-0.04982021
O	-0.07776375	-0.12872496	-5.23603340	C	0.21572432	6.88168347	-0.26568387
O	1.61870710	-5.77193396	-0.03936628	H	-0.72901232	7.37102013	-0.47615732
O	-1.07142068	-5.91031396	0.02194379	C	0.27655714	5.49189193	-0.23328567

H	-0.59520360	4.87624356	-0.41845851	H	3.71494383	2.63144286	3.64965588
N	-2.79011007	3.27471357	-2.84331306	C	5.49344220	1.98725757	4.70914839
C	-2.98576521	2.86239086	-4.11202656	H	5.44475255	2.78022092	5.44749782
H	-2.78495334	1.81552150	-4.30498689	C	6.51453929	1.03650528	4.72782826
C	-3.40566808	3.72643736	-5.11866242	H	7.28743267	1.07064514	5.48941294
H	-3.54983429	3.34625943	-6.12418450	C	6.52493492	0.04126835	3.74957245
C	-3.63026222	5.06803567	-4.80867660	H	7.29904176	-0.71788883	3.72266347
H	-3.95577230	5.76606416	-5.57373755	C	5.51518086	0.02821007	2.79257884
C	-3.43073039	5.49389899	-3.49548674	H	5.47087242	-0.73166272	2.02171074
H	-3.59500367	6.52563058	-3.20392968	H	-0.08787405	-0.69560273	-0.84951508
C	-3.01548662	4.56910535	-2.54266371	H	0.14719785	-0.69896347	0.84726696
H	-2.86318470	4.84524773	-1.50658705	H	0.21524510	2.37489957	-2.25688822
N	4.52976172	0.94684238	2.77606541	H	-0.13134332	3.53864627	1.84011409
C	4.52159191	1.91145575	3.71644061				

B3LYP-6-31G* (C, H, O, N, Na)/LanL2DZ (Mo)-optimized geometry of 5.

Total electronic charge: 0.

Mo	-2.34140755	2.04822313	2.22093975	O	2.94805266	2.78252614	-3.30383862
Mo	-3.41476425	2.70153137	0.00549821	O	4.28563498	2.05979868	-0.79976425
Mo	-1.09877213	3.62367169	0.57220878	O	1.66399476	-1.06855957	1.00403928
Mo	1.27582526	3.11151053	-2.18560352	O	4.67418469	-1.25023076	0.52370302
Mo	2.58353621	2.70899518	-0.03687958	O	3.70514733	-2.05818432	3.11902540
Mo	3.09871385	1.31081201	-2.11993144	O	3.12659468	-3.76464438	0.87220975
Mo	3.46826396	-0.58880743	1.88004073	O	-1.36399258	-1.91546539	-0.33723392
Mo	3.03660744	-2.13428572	-0.11496545	O	-1.71607835	-4.93894721	0.06779893
Mo	2.10177268	-2.69914020	2.19806300	O	-3.56740881	-3.62632462	-1.67009808
Mo	-0.38559004	-3.72206496	-0.66747439	O	-0.85111294	-4.01468637	-2.53057325
Mo	-2.81163127	-3.33889635	0.10202943	O	0.09052617	0.12914226	-5.83178089
Mo	-2.05725188	-2.52183953	-2.17732610	O	2.09281362	-2.63000525	-4.12387275
Mo	0.03018789	0.35508177	-4.13652945	O	-0.46118901	-1.30080894	-3.05073852
Mo	1.53905795	-1.52130702	-2.95072150	O	1.97020180	0.25348020	-3.70514496
Mo	0.40080698	-0.27091253	4.18253218	O	0.52228104	-0.00482876	5.86605062
Mo	1.42802677	1.86009875	2.89801176	O	1.83892752	3.07547181	4.02773274
Mo	-3.34126444	0.87341031	-2.92520722	O	-0.46484125	1.18546881	3.04705570
Mo	-5.38036809	-0.56900906	0.08875523	O	2.24189955	0.19298630	3.60659186
Mo	-2.78683113	-1.52123082	3.15905903	O	-4.85618198	0.94262968	-3.75105295
Na	-0.11490595	-0.00022327	0.07251583	O	-2.07927228	0.81438224	-4.20160903
O	-1.65738383	1.64349182	0.29349919	O	-4.26990545	-1.89593062	3.96667768
O	-4.10686329	2.70531888	1.83942354	O	-1.52696384	-1.18904893	4.39289305
O	-1.46796851	3.72882719	2.52901613	O	-2.29856495	-2.97885648	2.14040120
O	-2.76378998	4.51481110	0.05907938	O	0.94167958	2.91924227	1.27136474
O	1.34384246	1.37987091	-1.04293075	O	-2.96898597	0.05485229	2.29588893
O	2.41651555	4.31088349	-1.00650310	O	0.18157397	2.14566374	-3.59445758

O	-0.25836979	3.71735893	-1.13027822	H	-0.50087578	5.66334747	2.92429301
O	2.92627552	1.39142939	1.63123920	N	0.98605752	4.91722519	-3.49630449
O	-3.14077119	2.47463492	-2.05186776	C	2.01102417	5.73988905	-3.79114301
O	-4.47589088	0.92386985	-0.52617922	H	2.96470879	5.48844608	-3.34299963
O	-4.21603954	-1.91266984	0.59176910	C	1.86000220	6.84698156	-4.62090643
O	0.85664372	-2.03585877	3.60181067	H	2.71482718	7.48099120	-4.83077296
O	-6.36448441	-0.15638882	1.45952870	C	0.60348574	7.11621250	-5.16551622
O	-6.42323764	-1.15833672	-1.17220090	H	0.45493544	7.97252300	-5.81617227
O	2.98885718	-0.80213773	-1.76629782	C	-0.45823529	6.26436699	-4.85824205
O	0.36166849	-3.62752878	1.33422485	H	-1.45277143	6.43314437	-5.25694246
O	-3.16213939	-0.82544954	-2.23870731	C	-0.22733794	5.17606165	-4.02186748
O	1.35296753	-2.67732850	-1.27719909	H	-1.01772871	4.48315174	-3.75885395
N	-3.00439939	2.21880654	4.37256031	N	3.86751992	4.06561726	1.27082527
C	-2.18988266	2.74760308	5.30590888	C	5.10158264	3.68740679	1.65199533
H	-1.22239571	3.08589390	4.95556533	H	5.42944938	2.71832766	1.29862633
C	-2.56681139	2.86317528	6.64074399	C	5.91502407	4.49252645	2.44412669
H	-1.87691255	3.29630819	7.35703027	H	6.90344779	4.14522507	2.72414832
C	-3.83347805	2.42127887	7.02535388	C	5.43451763	5.73485541	2.86093012
H	-4.15630921	2.50021449	8.05886536	H	6.04462074	6.38441413	3.48109267
C	-4.67916803	1.87944894	6.05612050	C	4.15608250	6.12745666	2.46257686
H	-5.67415761	1.52704882	6.30575516	H	3.73854412	7.08366249	2.75880603
C	-4.22930299	1.79536944	4.74208371	C	3.40668647	5.26653230	1.66585719
H	-4.84885213	1.38295938	3.95482222	H	2.41344048	5.52948902	1.32582389
N	-5.37884316	3.73664124	-0.46414449	N	5.00075186	0.89397470	-3.31475030
C	-5.74321111	4.81152435	0.26325814	C	6.22436320	1.04603645	-2.77020235
H	-5.05360610	5.11866690	1.03982919	H	6.23991678	1.34631669	-1.72906079
C	-6.93265504	5.49647878	0.03677040	C	7.39317212	0.84076902	-3.49785383
H	-7.18171946	6.35505977	0.65109648	H	8.35540279	0.97296329	-3.01482932
C	-7.78071736	5.05870504	-0.98091499	C	7.29745068	0.47255090	-4.84047233
H	-8.71556326	5.57277143	-1.18213680	H	8.19136181	0.30870308	-5.43438602
C	-7.40339472	3.94712042	-1.73414194	C	6.03035645	0.32139187	-5.40590189
H	-8.02829235	3.56817083	-2.53578066	H	5.90505156	0.03897187	-6.44566518
C	-6.19793376	3.31265179	-1.44623853	C	4.90804099	0.54106889	-4.61270564
H	-5.87338856	2.44413196	-2.00438128	H	3.90248268	0.43226122	-5.00258009
N	-0.35972082	5.77546865	0.86960748	N	5.34110917	0.19652156	2.90022001
C	-0.08583905	6.54440722	-0.20176325	C	6.54595570	0.16946114	2.29730928
H	-0.17779890	6.05607854	-1.16296655	H	6.55914121	-0.22802912	1.28916272
C	0.30320604	7.87613352	-0.08477419	C	7.70372821	0.61288277	2.93033807
H	0.50962769	8.45435359	-0.97917131	H	8.65098496	0.57366530	2.40328161
C	0.42008137	8.43739404	1.18718431	C	7.61754328	1.09495686	4.23699343
H	0.72349004	9.47257613	1.31031412	H	8.50396973	1.44378151	4.75776395
C	0.13651226	7.64114199	2.29753822	C	6.37024430	1.11807969	4.86229225
H	0.20999410	8.03113906	3.30711021	H	6.25273451	1.48174057	5.87745158
C	-0.25427414	6.31976513	2.09870996	C	5.25715495	0.66226463	4.16254770

H	4.26641948	0.66173033	4.60278060	H	2.71706182	-8.97936669	-1.25456533
N	4.44551880	-3.31230513	-1.50178486	C	1.87947106	-7.27120010	-2.28004169
C	4.51005315	-4.65763414	-1.45178936	H	2.15751172	-7.59397965	-3.27757499
H	3.84293494	-5.13320172	-0.74500089	C	1.19609146	-6.07042908	-2.11201985
C	5.38928001	-5.39342405	-2.24082613	H	0.91938081	-5.44775971	-2.95372123
H	5.39477779	-6.47557570	-2.16830193	N	-4.40152245	-4.79326566	0.78172645
C	6.24801049	-4.71716142	-3.10740099	C	-5.21391640	-4.51864127	1.82114382
H	6.94877780	-5.26296923	-3.73172567	H	-5.07403376	-3.56027032	2.30553500
C	6.18872586	-3.32409926	-3.15312172	C	-6.18899675	-5.41224572	2.25572766
H	6.83646887	-2.75049061	-3.80698743	H	-6.81814336	-5.14751643	3.09878750
C	5.27372485	-2.66086407	-2.34044742	C	-6.33528674	-6.63071566	1.59287152
H	5.17661409	-1.58423760	-2.35390592	H	-7.08860834	-7.34582462	1.90878529
N	2.33428178	-4.49898164	3.54097201	C	-5.49473652	-6.91255297	0.51539049
C	3.46666037	-5.22905473	3.51090877	H	-5.57051655	-7.84547680	-0.03274757
H	4.22530174	-4.90286581	2.80979468	C	-4.54099604	-5.97142468	0.14169111
C	3.65461088	-6.34234041	4.32398902	H	-3.86393080	-6.14910292	-0.68473135
H	4.58508148	-6.89701426	4.26706365	N	-2.77415013	-2.86778053	-4.28952991
C	2.63380739	-6.72117766	5.19694363	C	-4.06628967	-2.65779327	-4.60996527
H	2.75074147	-7.58639881	5.84222928	H	-4.71126795	-2.33140592	-3.80300900
C	1.46110005	-5.96571173	5.22617047	C	-4.54936377	-2.84243028	-5.90152227
H	0.64094267	-6.21915377	5.88924329	H	-5.59815802	-2.66367523	-6.11237718
C	1.35071545	-4.86070803	4.38733344	C	-3.66604555	-3.25731478	-6.89956511
H	0.47143332	-4.22755437	4.38750796	H	-4.01346548	-3.40829261	-7.91695880
N	0.82442720	-5.61856812	-0.89807673	C	-2.32925868	-3.47784460	-6.56540878
C	1.12484915	-6.35412275	0.18991856	H	-1.60717886	-3.80539437	-7.30557419
H	0.81412881	-5.93574919	1.13895799	C	-1.92206886	-3.27532976	-5.25015283
C	1.80387392	-7.56609958	0.10188762	H	-0.89831650	-3.44358536	-4.93870339
H	2.02177976	-8.12458298	1.00595449	H	-0.41210725	-3.34985205	1.87486571
C	2.18834855	-8.03639903	-1.15457836				

B3LYP-6-31G* (C, H, O, N, P)/LanL2DZ (Mo, Zn)-optimized geometry of **6**.

Total electronic charge: -2.

Zn	-1.61614702	-2.47276013	-0.17195011	Mo	4.32587470	-2.70246145	0.02420526
Mo	-4.08625930	-0.31981760	1.28177086	Mo	4.84921079	0.18562634	-1.75119539
Mo	-2.69748134	1.50062129	0.07729868	Mo	4.93306625	0.28616354	1.67950625
Mo	-4.10918671	-0.22647093	-1.23754588	P	1.79982458	-0.03780829	-0.01402641
Mo	0.98559766	-3.12764393	1.70346529	P	-4.51962036	-3.21737875	-0.08870211
Mo	1.46334654	0.06834195	-3.54100033	P	-1.47309546	-1.50766561	3.24272071
Mo	1.10959289	-2.93580408	-1.98732451	P	-1.54151531	-1.32709992	-3.37567934
Mo	0.49765476	3.08973505	-1.57443392	O	-2.48277863	-0.63060800	-0.00402212
Mo	0.62424406	2.87875673	1.87362719	O	-5.55102886	0.02499918	0.02648986
Mo	3.54029822	3.18311257	0.01119864	O	-3.88487348	1.64188753	1.54677417
Mo	1.61993621	-0.33593347	3.49596937	O	-3.88569366	1.73702973	-1.38763625

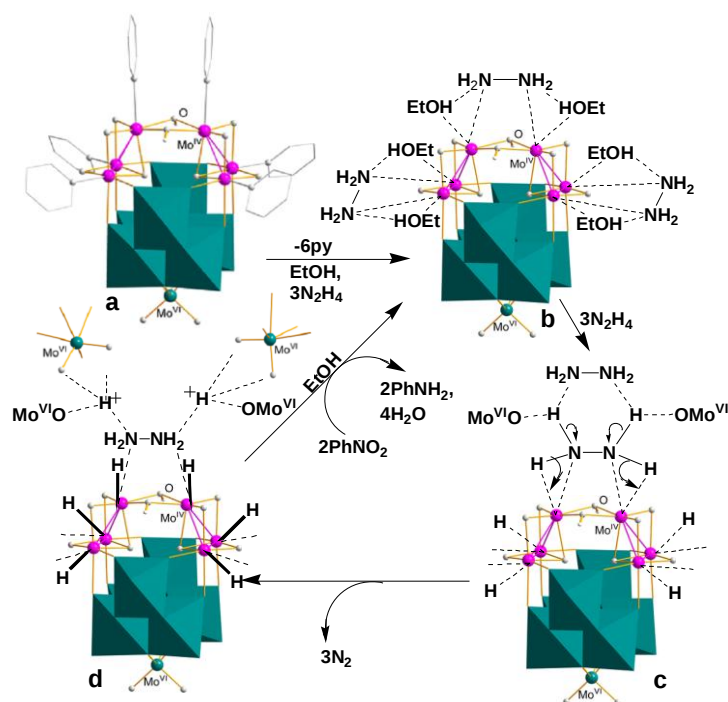
O	-4.60019111	-2.17679382	-1.32778518	O	1.28950721	1.77653398	-2.83828119
O	-4.61662809	-2.26225115	1.21216665	O	0.37676938	-3.17675694	-0.15085257
O	-3.06682300	-3.80165633	-0.09990181	O	0.71669823	-4.70785780	2.25836378
O	-5.62350566	-4.23108942	-0.13139926	O	2.79468958	-3.07034264	-1.35079135
O	-0.87957517	-2.17180333	-2.17244624	O	1.80335619	-0.15095899	5.17456387
O	-2.77116630	-0.54237313	-2.85082742	N	-5.66926373	-0.15323664	2.84706108
O	-0.45705244	-0.09566671	-3.59735836	C	-5.44756254	0.56680457	3.96408047
O	-1.71383789	-2.11641184	-4.62955500	H	-4.48859189	1.06608438	4.03036436
O	-0.92870027	-2.36790415	1.96447441	C	-6.39383946	0.66807319	4.97788504
O	-2.79123109	-0.77813817	2.83309144	H	-6.17292770	1.25865318	5.86015526
O	-0.41342428	-0.28442676	3.36192260	C	-7.61253922	0.00447384	4.83134942
O	-1.55991747	-2.34269164	4.47829149	H	-8.37082466	0.06544956	5.60576034
O	-0.95305989	1.66164295	1.45380493	C	-7.84027096	-0.73774326	3.67202442
O	-1.02531541	1.76730391	-1.42168570	H	-8.77255539	-1.26886318	3.51418072
O	1.28189619	1.60327174	2.99064542	C	-6.84515923	-0.79415114	2.70225954
O	5.13052231	-1.72515904	-1.36996280	H	-6.96691726	-1.36067919	1.78798954
O	2.28799266	3.77020839	-1.29018261	N	-2.89759721	3.73390900	0.15663962
O	5.06187778	-1.80611051	1.41414553	C	-2.94789455	4.37127267	1.34334010
O	3.35098290	-0.20649593	2.88739034	H	-2.85499089	3.75024758	2.22488789
O	3.35239484	-0.37539797	-0.01319123	C	-3.12250746	5.74756762	1.43858157
O	6.18965690	0.48386702	-2.75004910	H	-3.15764822	6.21525992	2.41630924
O	2.24114688	3.72569423	1.37997738	C	-3.25766054	6.49462355	0.26793868
O	0.83103243	-4.45541265	-2.69142296	H	-3.39881661	7.56999231	0.31137899
O	-0.14491029	4.24434454	-2.63408078	C	-3.21692083	5.83206923	-0.95942296
O	5.83699122	0.32433199	0.08761489	H	-3.32781825	6.36674601	-1.89635968
O	1.66268711	1.52551772	0.04924855	C	-3.03933489	4.45301587	-0.97483269
O	1.16441649	-0.71879606	1.21562955	H	-3.02035160	3.89403249	-1.90147526
O	6.15421324	0.46209105	2.84592802	N	-5.69232935	0.03056153	-2.79007434
O	4.23214947	1.98549127	1.46097043	C	-5.48579332	0.84283936	-3.84511950
O	4.63403198	4.47290194	0.08576753	H	-4.54479650	1.37884511	-3.85993938
O	1.49311362	-1.87225990	-3.52070880	C	-6.42502838	0.98864557	-4.85998561
O	-0.01194120	3.65045228	0.08111537	H	-6.21639337	1.65188756	-5.69216493
O	3.45153242	0.00215340	-2.89119444	C	-7.62080666	0.27408207	-4.77986410
O	2.72885080	-3.19419053	1.14812632	H	-8.37260814	0.36728488	-5.55736703
O	1.87531615	0.36436150	-5.16129132	C	-7.83438641	-0.56123618	-3.68286973
O	-0.07496760	4.02583899	2.90849605	H	-8.74908754	-1.13426525	-3.57766144
O	5.15235125	-4.18131367	-0.01324210	C	-6.84728002	-0.65814579	-2.70821085
O	1.19138529	-0.60140784	-1.32258233	H	-6.95765734	-1.29832972	-1.84234929
O	4.36853964	1.99411635	-1.20097950	H	-0.89991724	0.89633661	2.08724525
O	1.40208561	-2.21515487	3.35806367	H	-1.09545727	1.14725492	-2.18124926

B3LYP-6-31G* (C, H, O, N)/LanL2DZ (Mo)-optimized geometry of **7**.

Total electronic charge: -2.

Mo	1.04707937	1.03531385	-0.28489616	H	5.32815808	2.24713741	2.59274738
Mo	0.37224931	-1.42410064	-0.28319522	C	3.53391134	1.87599119	1.48593252
Mo	-1.42141451	0.38919748	-0.28706355	H	3.83440521	0.89552168	1.13659056
O	-0.00026553	-0.00031815	-1.74602094	C	4.81177331	4.77116123	3.60200727
O	-0.43486319	1.65617745	0.81170650	H	5.48074507	4.17112729	4.22594519
O	1.64663205	-0.44983067	0.81774447	H	4.21628161	5.42325055	4.24783188
O	-1.21639943	-1.20075584	0.81594016	H	5.43879285	5.41548905	2.97213566
O	2.78416676	0.94564939	-1.47144074	C	2.08896686	-3.40760469	1.49363725
O	0.98593790	2.76552357	-1.47902425	H	2.84499516	-2.71218522	1.14924647
O	2.03243851	3.99135211	-3.05171420	C	2.41173815	-4.48409978	2.30902620
O	4.02872870	1.97146187	-3.04350779	H	3.44548103	-4.63514467	2.60411276
O	1.90787324	-2.23030056	-1.47307039	C	1.40680180	-5.35893921	2.74472055
O	-0.56534818	-2.88438975	-1.47260596	C	0.09896819	-5.07883362	2.32708317
O	-0.28988401	-4.47639319	-3.04184842	H	-0.72928905	-5.70861758	2.63645439
O	2.45239718	-3.73914451	-3.05396859	C	-0.14972131	-3.98274259	1.51075931
O	-2.88769558	-0.53630994	-1.47878971	H	-1.15259141	-3.73967815	1.18063499
O	-2.21236365	1.93113022	-1.48034465	C	1.72268784	-6.55367391	3.60464206
O	-3.72196362	2.49028417	-3.05549561	H	2.01557279	-7.40533166	2.97706684
O	-4.46969408	-0.25052806	-3.05539114	H	0.85504701	-6.86189145	4.19506488
N	2.31745642	2.29727367	1.09002085	H	2.55594249	-6.34660574	4.28308633
N	0.82777080	-3.15647060	1.09227365	C	-3.38242411	2.12321996	1.49759269
N	-3.15192511	0.86235330	1.08355269	H	-2.67088882	2.87006585	1.16644984
C	3.04383957	1.90051867	-2.31940112	C	-4.46182301	2.45710646	2.30498071
C	1.94753440	3.01055280	-2.32361698	H	-4.60040965	3.49103274	2.60543434
C	1.64354364	-3.18256996	-2.32232811	C	-5.35802003	1.46358352	2.72254839
C	0.13594607	-3.58462454	-2.31888151	C	-5.10308153	0.15661570	2.28611852
C	-3.57981740	0.17026765	-2.32727325	H	-5.75755827	-0.66110873	2.57154596
C	-3.16813461	1.67532460	-2.32831699	C	-4.00300182	-0.10355015	1.47913288
C	1.89213361	3.50309162	1.51357473	H	-3.77974875	-1.10558307	1.13281550
H	0.90225336	3.79959272	1.18803901	C	-6.52403670	1.78202250	3.62024826
C	2.66276378	4.32069232	2.32990548	H	-7.34324584	1.07127454	3.47767446
H	2.26703901	5.28140920	2.64433780	H	-6.89923649	2.79419721	3.44188613
C	3.93453414	3.90047173	2.74238374	H	-6.21813986	1.72620900	4.67307301
C	4.35880251	2.63962366	2.30153319				

9. The proposed catalytic cycle reported in our previous work⁶



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