

## Supporting Information for

# Unveiling the catalytic potency of copper-integrated $[P_6Mo_{18}O_{73}]^{n-}$ -based complex: structural basis and enhanced performance in selective oxidation of aromatic alcohol

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### 1. Materials and general methods.

All chemicals were commercially purchased without further purification. Sodium molybdate dihydrate ( $\geq 99.0\%$ ), Phosphoric acid ( $\geq 85.0\%$ ), Copper(II) chloride dihydrate ( $\geq 99.0\%$ ), Strontium chloride hexahydrate ( $\geq 99.0\%$ ), Sodium hydroxide ( $\geq 96.0\%$ ), Hydrochloric acid ( $\geq 36.0\text{--}38.0\%$ ), Benzimidazole ( $\geq 99.0\%$ ), Ethanol ( $\geq 99.7\%$ ), Acetonitrile ( $\geq 99.0\%$ ), Ethyl acetate ( $\geq 99.5\%$ ), Cyclohexane ( $\geq 99.5\%$ ), tert-Butyl hydroperoxide ( $\geq 70\%$ ), All catalytic reaction substrates were purchased from Shanghai Aladdin Biochemical Technology Co., Ltd., with a purity of  $\geq 97.0\%$ . The powder X-ray diffraction (PXRD) patterns were measured using a D/teX Ultra diffractometer. Fourier transform infrared spectra (FT-IR) were conducted on a Varian 640 FTIR spectrophotometer using KBr pellets in  $400 - 4000\text{ cm}^{-1}$ . X-ray photoelectron spectrum (XPS) was measured using a Thermomo Scientific K-Alpha photo-electron spectrometer. The Raman spectroscopy was measured using a high-resolution confocal micro Raman spectrometer. The catalytic reaction was analyzed using a Shimadzu gas chromatograph (GC) GC-2010 Pro with a flame ionization detector equipped with a TM-5 Sil capillary column.

### 2. X-ray crystallography.

The crystallographic data of the complex were acquired using a Bruker D8 QUEST diffractometer equipped with a Bruker APEX-II CCD detector and graphite-

monochromated Mo K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 296.15 K. Absorption corrections were applied using the multi-scan program SADABS. The structure was solved by direct methods using the ShelXT program with intrinsic phasing and refined by full-matrix least-squares methods on  $F^2$  using the ShelXL 2018/3 program.[1,2] All non-hydrogen atoms were refined anisotropically, while hydrogen atoms were refined isotropically. The guest water molecules are severely disordered and therefore removed using the “Solvent Mask” program in the Olex2 software package. The crystallographic data for complexes **1** and **2** can be obtained free of charge from the Cambridge Crystallographic Data Centre via <https://www.ccdc.cam.ac.uk/structures/>. (CCDC numbers: 2474578 and 2474579)

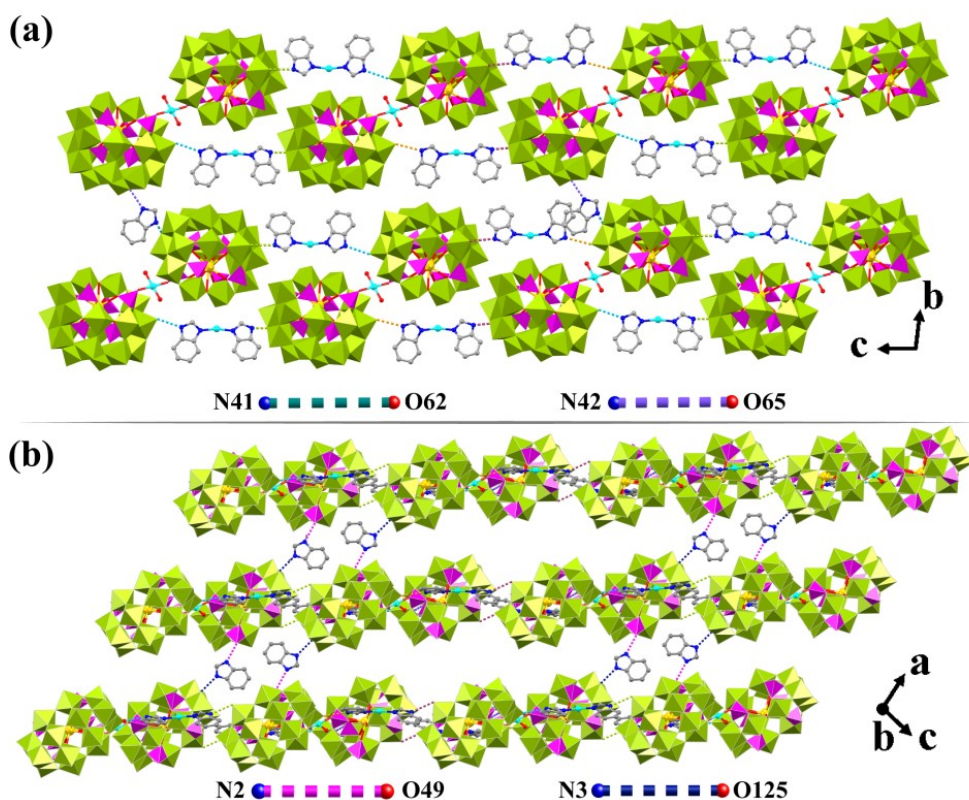


Fig. S1 (a) The 2D supramolecular layered structure of complex **1**, (b) the 3D supramolecular framework structure of complex **1**.

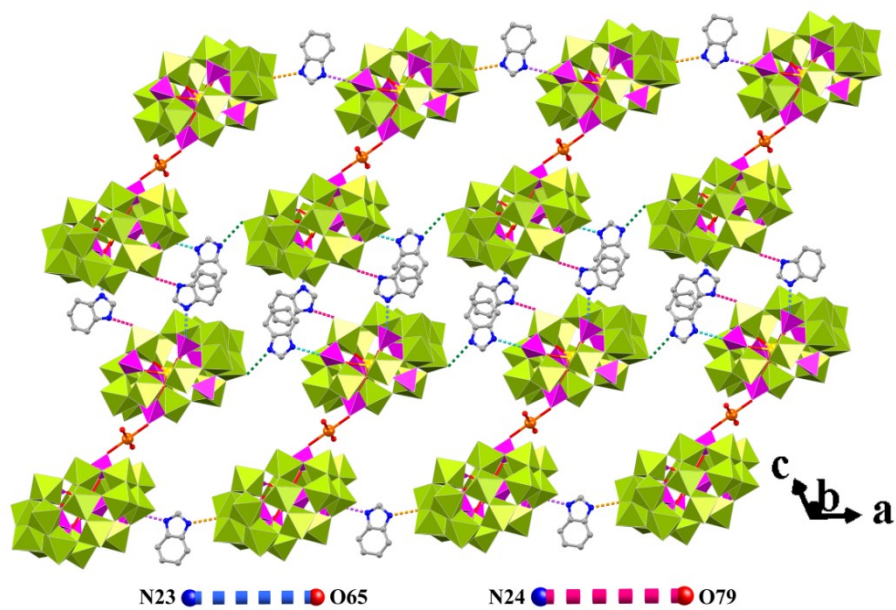


Fig. S2 The 2D supramolecular layered structure of complex 2.

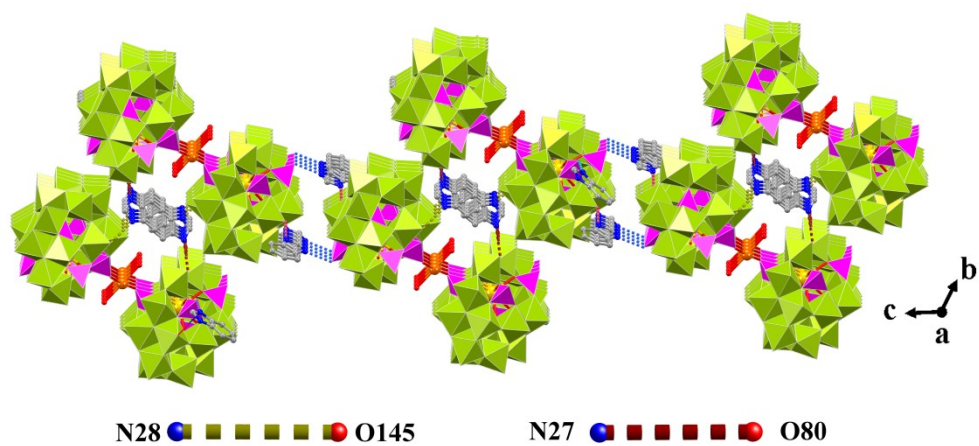


Fig. S3 The 3D supramolecular framework structure of complex 2.

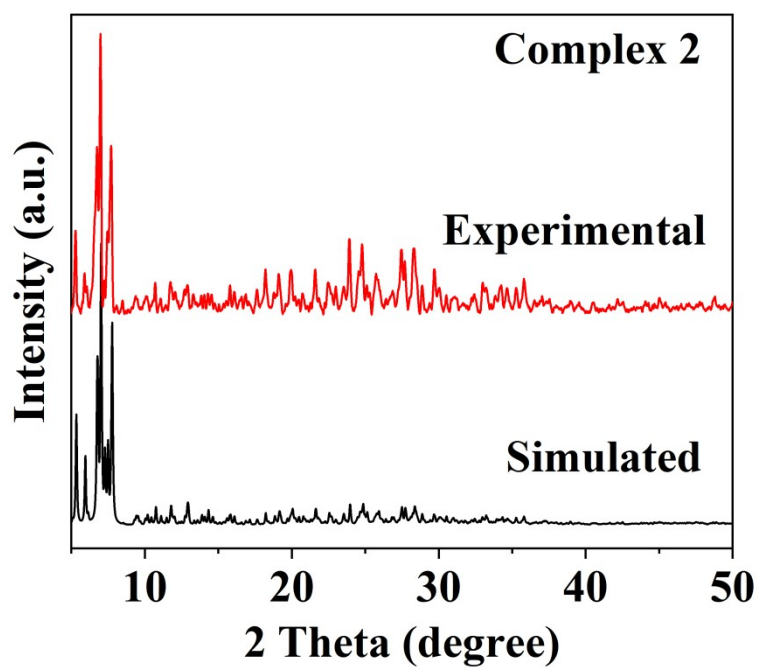


Fig. S4 The PXRD patterns of complex 2.

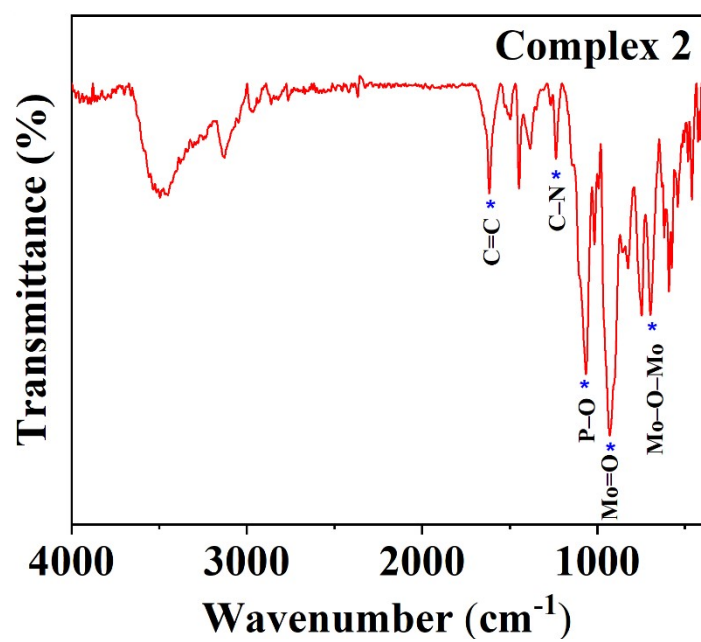


Fig. S5 The FT-IR spectrum of complex 2.

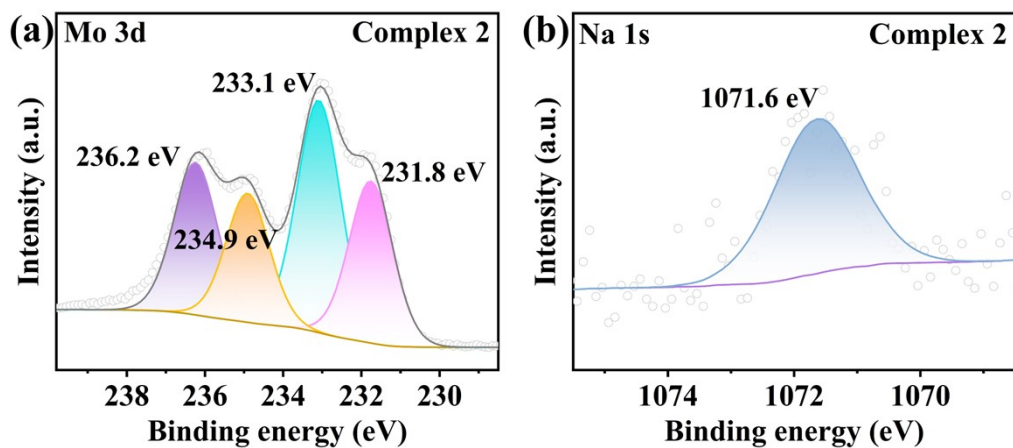
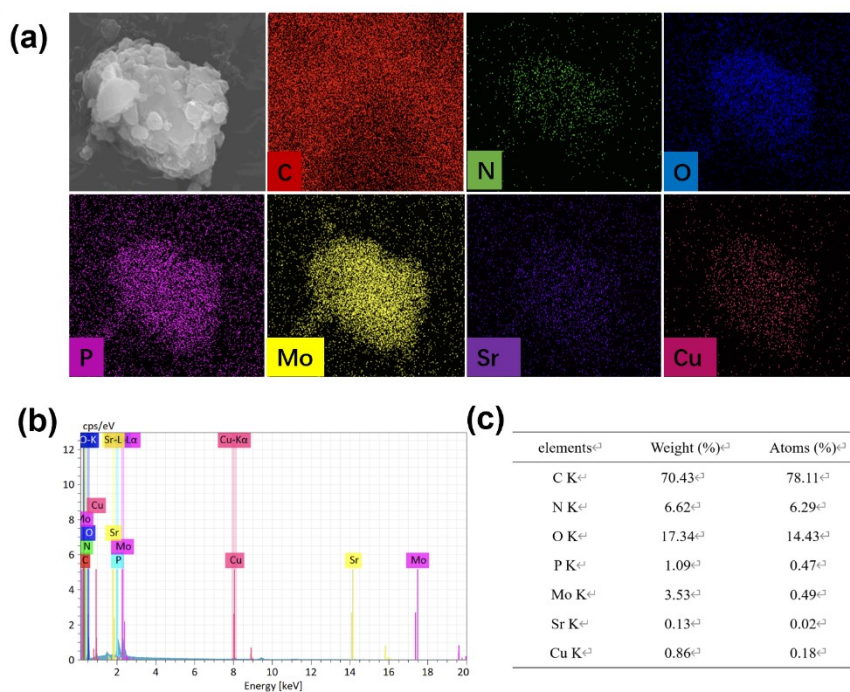


Fig. S6 XPS spectra of (a) Mo 3d and (b) Na 1s in complex 2.



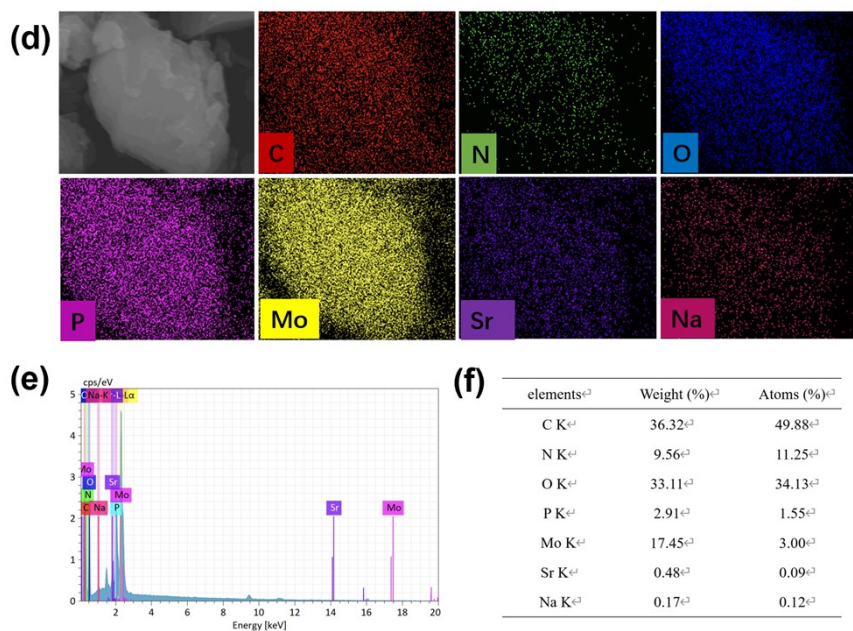


Fig. S7 SEM-EDS characterization of the complex 1: (a) elemental mapping, (b) spectrum, and (c) quantitative data. SEM-EDS characterization of the complex 2: (d) elemental mapping, (e) spectrum, and (f) quantitative data.

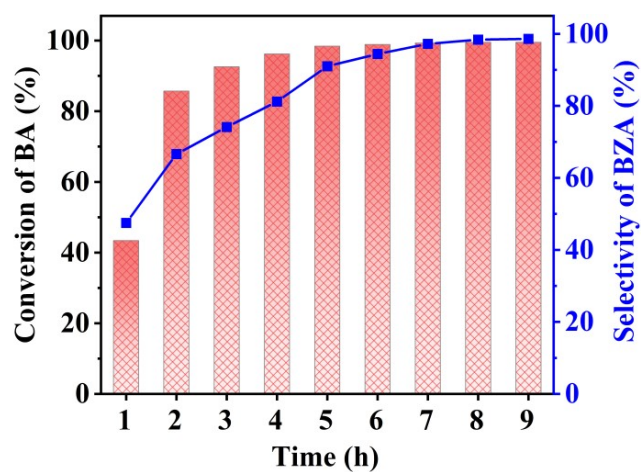


Fig. S8 The change of BA catalytic oxidation over time for complex 1.

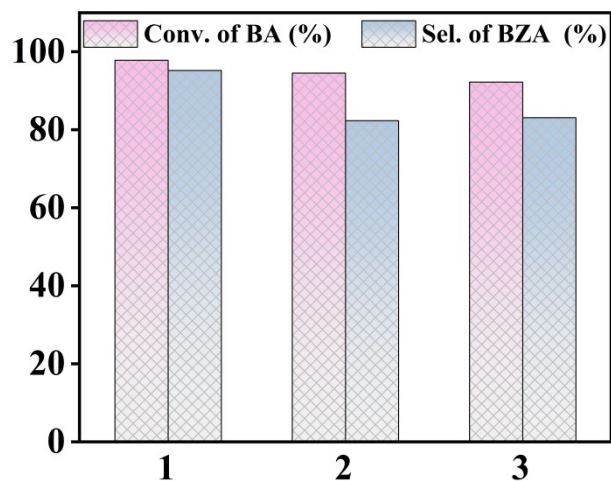


Fig. S9 Cyclic experiment of complex 1 as a catalyst.

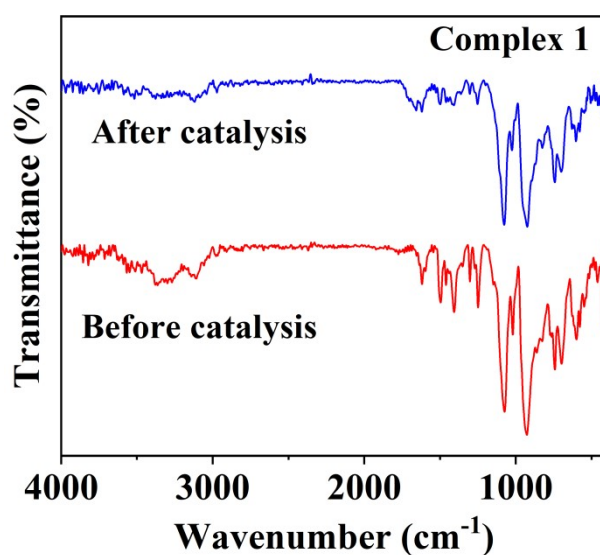


Fig. S10 IR spectra of complex 1 before and after catalyzing the reaction.

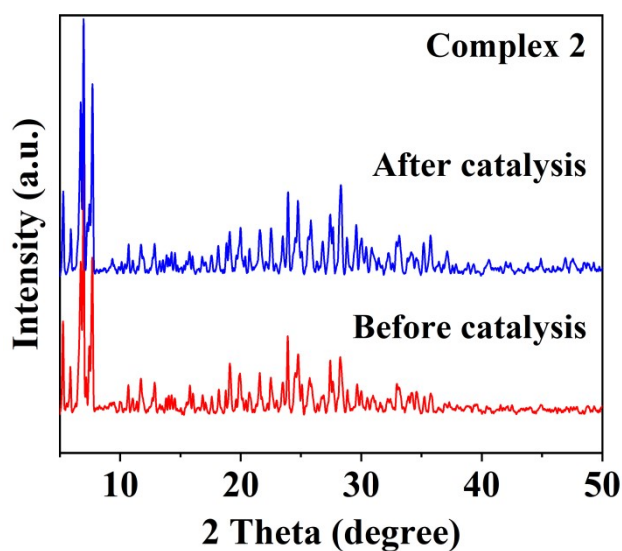


Fig. S11 PXRD patterns of complex 2 before and after catalyzing the reaction.

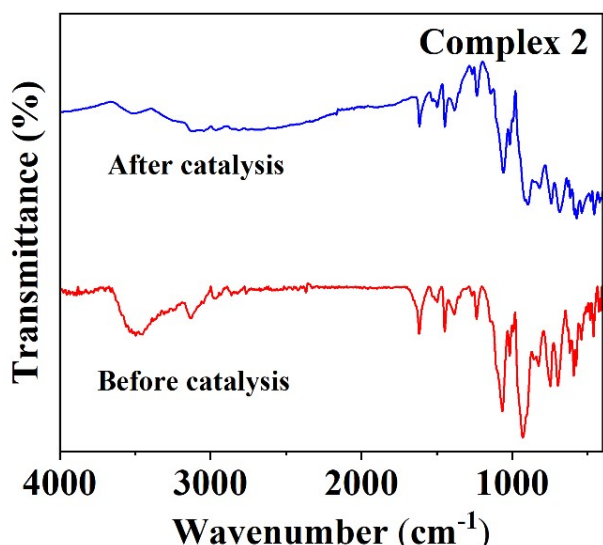


Fig. S12 FT-IR spectra of complex 2 before and after the catalytic reaction.

Table S1. Crystal data and structure refinement for complexes 1 and 2.

Crystal Data	Complex 1	Complex 2
Empirical formula	C <sub>154</sub> H <sub>208</sub> Cu <sub>9</sub> Mo <sub>36</sub> N <sub>88</sub> O <sub>183</sub> P <sub>12</sub> Sr <sub>2</sub>	C <sub>259</sub> H <sub>321</sub> Mo <sub>72</sub> N <sub>74</sub> Na <sub>2</sub> O <sub>324</sub> P <sub>24</sub> Sr <sub>4</sub>
Formula weight	10176.21	17702.30
Temperature/K	296.15	296.15
Crystal system	triclinic	triclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$
<i>a</i> (Å)	17.8685(8)	18.3207(5)
<i>b</i> (Å)	20.0947(9)	26.9821(8)
<i>c</i> (Å)	42.1985(19)	28.8827(9)
$\alpha$ (Å)	97.054(2)	116.8600(10)
$\beta$ (Å)	100.416(2)	94.4990(10)
$\gamma$ (Å)	91.774(2)	104.0350(10)
Volume(Å <sup>3</sup> )	14767.4(12)	12061.9(6)
<i>Z</i>	2	1
<i>D<sub>c</sub></i> (g cm <sup>3</sup> )	2.289	2.437
$\mu$ (mm <sup>-1</sup> )	2.636	2.438
<i>F</i> (000)	9866.0	8543.0
Reflections collected	544505	564785
Independent reflections	51930	47444
Data/restraints/parameters	51930/1071/3679	47444/634/3390
GoF	1.054	1.019
R indexes [ <i>I</i> ≥ 2σ ( <i>I</i> )]	R <sub>1</sub> = 0.0742, wR <sub>2</sub> = 0.1963	R <sub>1</sub> = 0.0306, wR <sub>2</sub> = 0.0777
R [all data]	R <sub>1</sub> = 0.0834, wR <sub>2</sub> = 0.2002	R <sub>1</sub> = 0.0355, wR <sub>2</sub> = 0.0806

$R_1 = \Sigma ||F_o| - |F_c| || / \Sigma |F_o|$ ;  $wR_2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$

Table S2. The bond lengths (Å) in complex 1.

Mo1–O12	2.045(7)	Mo15–O63	2.171(7)	Mo29–O98	1.923(7)
Mo1–O15	2.290(7)	Mo15–O83	1.775(7)	Mo29–O102	1.664(8)

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Mo1-O21	1.828(7)	Mo15-O91	1.787(7)	Mo30-O17	2.300(7)
Mo1-O38	2.325(6)	Mo15-O107	1.678(7)	Mo30-O48	1.979(9)
Mo1-O90	1.692(7)	Mo16-O24	2.278(7)	Mo30-O54	1.875(7)
Mo1-O99	1.724(7)	Mo16-O39	2.244(7)	Mo30-O66	2.087(7)
Mo2-O2	2.218(7)	Mo16-O53	2.012(8)	Mo30-O81	1.886(7)
Mo2-O14	2.022(7)	Mo16-O96	1.892(7)	Mo30-O137	1.700(7)
Mo2-O30	2.024(7)	Mo16-O131	1.699(8)	Mo31-O33	1.776(7)
Mo2-O59	1.893(7)	Mo16-O140	1.707(8)	Mo31-O47	2.418(7)
Mo2-O67	1.912(7)	Mo17-O40	1.815(7)	Mo31-O55	1.799(8)
Mo2-O112	1.666(8)	Mo17-O42	2.056(7)	Mo31-O56	2.060(7)
Mo3-O6	2.404(7)	Mo17-O63	2.323(7)	Mo31-O60	2.149(7)
Mo3-O12	2.044(7)	Mo17-O86	2.309(7)	Mo31-O126	1.702(8)
Mo3-O38	2.133(7)	Mo17-O104	1.700(8)	Mo32-O6	2.410(7)
Mo3-O44	1.800(8)	Mo17-O125	1.711(8)	Mo32-O44	2.105(8)
Mo3-O62	1.774(7)	Mo18-O43	2.283(6)	Mo32-O70	2.038(7)
Mo3-O93	1.698(7)	Mo18-O58	1.904(7)	Mo32-O74	1.788(7)
Mo4-O1	2.203(7)	Mo18-O80	2.115(7)	Mo32-O80	1.791(7)
Mo4-O9	2.054(7)	Mo18-O81	1.876(7)	Mo32-O145	1.695(8)
Mo4-O41	1.886(7)	Mo18-O98	1.918(9)	Mo33-O22	2.289(7)
Mo4-O59	1.841(7)	Mo18-O148	1.690(7)	Mo33-O77	1.881(7)
Mo4-O83	2.057(6)	Mo19-O28	1.776(7)	Mo33-O82	1.930(8)
Mo4-O97	1.699(7)	Mo19-O32	2.414(7)	Mo33-O94	2.100(7)
Mo5-O13	2.195(7)	Mo19-O42	2.060(7)	Mo33-O101	1.867(8)
Mo5-O19	2.040(7)	Mo19-O78	1.807(8)	Mo33-O141	1.692(8)
Mo5-O52	1.837(7)	Mo19-O86	2.143(7)	Mo34-O31	2.282(7)
Mo5-O58	1.882(7)	Mo19-O127	1.692(8)	Mo34-O65	1.957(7)
Mo5-O62	2.079(7)	Mo20-O32	2.428(7)	Mo34-O73	2.105(7)
Mo5-O103	1.690(7)	Mo20-O66	1.784(7)	Mo34-O76	1.872(8)
Mo6-O3	2.225(7)	Mo20-O78	2.070(9)	Mo34-O123	1.879(8)
Mo6-O36	2.017(7)	Mo20-O84	1.797(8)	Mo34-O142	1.699(8)
Mo6-O50	1.886(7)	Mo20-O91	2.103(7)	Mo35-O22	2.291(7)
Mo6-O68	2.026(7)	Mo20-O121	1.696(7)	Mo35-O82	1.931(8)
Mo6-O76	1.906(8)	Mo21-O45	2.148(8)	Mo35-O108	2.090(8)
Mo6-O136	1.663(7)	Mo21-O47	2.391(6)	Mo35-O110	1.889(8)
Mo7-O4	2.200(7)	Mo21-O56	2.057(8)	Mo35-O123	1.871(8)
Mo7-O29	2.043(8)	Mo21-O87	1.786(8)	Mo35-O139	1.681(8)
Mo7-O35	1.857(7)	Mo21-O124	1.790(8)	Mo36-O47	2.428(7)
Mo7-O72	2.061(7)	Mo21-O135	1.686(7)	Mo36-O55	2.082(9)
Mo7-O95	1.887(8)	Mo22-O11	2.230(7)	Mo36-O94	1.786(8)
Mo7-O113	1.677(7)	Mo22-O33	2.037(7)	Mo36-O108	1.798(9)
Mo8-O5	2.223(6)	Mo22-O35	1.873(7)	Mo36-O124	2.078(8)
Mo8-O28	2.028(7)	Mo22-O61	2.051(8)	Mo36-O143	1.688(8)
Mo8-O52	1.896(7)	Mo22-O101	1.898(8)	Sr1-O3	2.652(7)
Mo8-O54	1.887(7)	Mo22-O118	1.685(7)	Sr1-O4	2.686(6)

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Mo8–O64	2.049(7)	Mo23–O17	2.297(8)	Sr1–O10	2.580(7)
Mo8–O115	1.679(7)	Mo23–O41	1.898(7)	Sr1–O11	2.671(7)
Mo9–O7	2.229(7)	Mo23–O48	1.898(8)	Sr1–O16	2.686(7)
Mo9–O26	2.280(7)	Mo23–O84	2.098(8)	Sr1–O23	2.557(7)
Mo9–O40	2.007(7)	Mo23–O85	1.863(7)	Sr1–O24	2.582(7)
Mo9–O51	1.906(7)	Mo23–O109	1.657(8)	Sr1–O39	2.571(7)
Mo9–O114	1.700(7)	Mo24–O16	2.206(7)	Sr1–O96	2.873(8)
Mo9–O138	1.703(8)	Mo24–O37	2.049(7)	Sr2–O1	2.685(7)
Mo10–O8	2.194(7)	Mo24–O50	1.848(7)	Sr2–O2	2.650(7)
Mo10–O21	2.003(7)	Mo24–O87	2.049(7)	Sr2–O5	2.681(6)
Mo10–O27	2.273(7)	Mo24–O110	1.887(8)	Sr2–O7	2.599(7)
Mo10–O51	1.898(7)	Mo24–O119	1.697(7)	Sr2–O8	2.585(7)
Mo10–O117	1.699(7)	Mo15–O42	2.054(8)	Mo29–O74	2.085(7)
Mo10–O122	1.709(8)	Mo25–O45	2.325(7)	Mo29–O85	1.883(7)
Mo11–O6	2.444(6)	Mo25–O53	1.813(8)	Sr2–O13	2.666(7)
Mo11–O12	2.057(7)	Mo25–O56	2.052(8)	Sr2–O26	2.583(6)
Mo11–O15	2.115(7)	Mo25–O60	2.299(7)	Sr2–O27	2.588(7)
Mo11–O30	1.782(7)	Mo25–O128	1.705(7)	Sr2–O51	2.881(7)
Mo11–O70	1.820(7)	Mo25–O129	1.706(8)	Cu1–O1W	1.994(11)
Mo11–O89	1.671(7)	Mo26–O18	2.420(7)	Cu1–O2W	1.972(11)
Mo12–O20	2.305(7)	Mo26–O69	2.077(8)	Cu1–O57	1.892(7)
Mo12–O25	2.316(7)	Mo26–O73	1.805(8)	Cu1–O92	1.877(8)
Mo12–O34	1.835(7)	Mo26–O79	2.050(8)	Cu2–N5	1.877(10)
Mo12–O46	2.049(7)	Mo26–O88	1.781(8)	Cu2–N7	1.880(11)
Mo12–O100	1.722(7)	Mo26–O144	1.686(8)	Cu3–N8	1.878(11)
Mo12–O133	1.697(7)	Mo27–O10	2.190(7)	Cu3–N12	1.870(11)
Mo13–O18	2.378(7)	Mo27–O23	2.281(7)	Cu4–N22	1.916(12)
Mo13–O25	2.132(7)	Mo27–O34	1.986(7)	Cu4–N24	1.89(2)
Mo13–O46	2.045(7)	Mo27–O96	1.907(7)	Cu5–N34	1.86(3)
Mo13–O69	1.791(7)	Mo27–O130	1.713(8)	Cu5–N45	1.86(2)
Mo13–O72	1.780(7)	Mo27–O134	1.686(8)	Cu6–N19	1.896(13)
Mo13–O105	1.705(8)	Mo28–O31	2.290(7)	Cu6–N20	1.880(14)
Mo14–O18	2.431(7)	Mo28–O65	1.936(8)	Cu7–N28	1.878(16)
Mo14–O20	2.101(7)	Mo28–O77	1.880(7)	Cu7–N31	1.822(18)
Mo14–O46	2.054(7)	Mo28–O88	2.097(7)	Cu8–N13	1.862(11)
Mo14–O68	1.793(7)	Mo28–O95	1.880(8)	Cu8–N33	1.862(10)
Mo14–O79	1.810(8)	Mo28–O132	1.683(8)	Cu9–N38	1.868(15)
Mo14–O106	1.680(7)	Mo29–O43	2.322(8)	Cu9–N43	1.89(2)
Mo15–O32	2.414(6)	Mo29–O67	1.882(7)		

Table S3. The bond angles (°) in complex 1.

O12–Mo1–O15	69.2(2)	O83–Mo15–O91	101.0(3)	O41–Mo23–O48	157.1(3)
O12–Mo1–O38	69.2(2)	O91–Mo15–	75.9(3)	O41–Mo23–	88.3(3)

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		O32		O84	
O15-Mo1-O38	82.6(2)	O91-Mo15-O42	93.8(3)	O48-Mo23-O17	72.9(3)
O21-Mo1-O12	145.4(3)	O91-Mo15-O63	157.8(3)	O48-Mo23-O84	83.6(3)
O21-Mo1-O15	84.9(3)	O107-Mo15-O32	170.2(3)	O84-Mo23-O17	78.8(3)
O21-Mo1-O38	85.4(3)	O107-Mo15-O42	98.6(3)	O85-Mo23-O17	88.4(3)
O90-Mo1-O12	97.9(3)	O107-Mo15-O63	98.3(3)	O85-Mo23-O41	89.5(3)
O90-Mo1-O15	88.5(3)	O107-Mo15-O83	104.8(4)	O85-Mo23-O48	93.6(3)
O90-Mo1-O21	104.3(3)	O107-Mo15-O91	100.8(4)	O85-Mo23-O84	167.1(3)
O90-Mo1-O38	166.3(3)	O39-Mo16-O24	75.2(3)	O109-Mo23-O17	169.3(3)
O90-Mo1-O99	102.7(4)	O53-Mo16-O24	80.1(3)	O109-Mo23-O41	100.5(4)
O99-Mo1-O12	97.1(3)	O53-Mo16-O39	80.5(3)	O109-Mo23-O48	101.2(4)
O99-Mo1-O15	163.6(3)	O96-Mo16-O24	78.9(3)	O109-Mo23-O84	91.8(4)
O99-Mo1-O21	103.5(3)	O96-Mo16-O39	79.1(3)	O109-Mo23-O85	101.1(4)
O99-Mo1-O38	84.0(3)	O96-Mo16-O53	153.8(3)	O37-Mo24-O16	77.9(3)
O14-Mo2-O2	77.4(2)	O131-Mo16-O24	89.2(4)	O37-Mo24-O87	81.6(3)
O14-Mo2-O30	82.3(3)	O131-Mo16-O39	164.1(4)	O50-Mo24-O16	85.4(3)
O30-Mo2-O2	83.0(3)	O131-Mo16-O53	94.3(4)	O50-Mo24-O37	92.0(3)
O59-Mo2-O2	84.5(3)	O131-Mo16-O96	101.0(4)	O50-Mo24-O87	167.0(3)
O59-Mo2-O14	93.9(3)	O131-Mo16-O140	102.5(4)	O50-Mo24-O110	95.1(3)
O59-Mo2-O30	167.5(3)	O140-Mo16-O24	168.1(3)	O87-Mo24-O16	82.2(3)
O59-Mo2-O67	90.7(3)	O140-Mo16-O39	93.0(3)	O110-Mo24-O16	85.4(3)
O67-Mo2-O2	84.1(3)	O140-Mo16-O53	96.5(4)	O110-Mo24-O37	161.2(3)
O67-Mo2-O14	160.4(3)	O140-Mo16-	100.7(4)	O110-Mo24-	87.8(3)

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		O96		O87	
O67–Mo2–O30	89.1(3)	O40–Mo17– O42	144.8(3)	O119–Mo24– O16	171.1(3)
O112–Mo2–O2	174.2(3)	O40–Mo17– O63	85.1(3)	O119–Mo24– O37	94.7(3)
O112–Mo2– O14	97.4(3)	O40–Mo17– O86	84.3(3)	O119–Mo24– O50	99.9(3)
O112–Mo2– O30	94.0(3)	O42–Mo17– O63	69.1(3)	O119–Mo24– O87	91.9(3)
O112–Mo2– O59	98.3(3)	O42–Mo17– O86	69.6(3)	O119–Mo24– O110	101.2(4)
O112–Mo2– O67	100.8(4)	O86–Mo17– O63	83.2(3)	O53–Mo25– O45	85.6(3)
O12–Mo3–O6	73.3(2)	O104–Mo17– O40	104.3(3)	O53–Mo25– O56	145.7(3)
O12–Mo3–O38	73.3(3)	O104–Mo17– O42	97.9(3)	O53–Mo25– O60	84.5(3)
O38–Mo3–O6	83.7(2)	O104–Mo17– O63	86.6(3)	O56–Mo25– O45	69.3(3)
O44–Mo3–O6	75.8(3)	O104–Mo17– O86	166.1(3)	O56–Mo25– O60	70.2(3)
O44–Mo3–O12	93.5(3)	O104–Mo17– O125	101.9(4)	O60–Mo25– O45	83.4(3)
O44–Mo3–O38	158.2(3)	O125–Mo17– O40	104.0(4)	O128–Mo25– O45	85.6(3)
O62–Mo3–O6	84.3(3)	O125–Mo17– O42	97.6(3)	O128–Mo25– O53	104.1(4)
O62–Mo3–O12	150.3(3)	O125–Mo17– O63	165.2(3)	O128–Mo25– O56	97.1(3)
O62–Mo3–O38	85.4(3)	O125–Mo17– O86	86.2(3)	O128–Mo25– O60	165.5(4)
O62–Mo3–O44	99.7(3)	O58–Mo18– O43	84.1(3)	O128–Mo25– O129	102.5(4)
O93–Mo3–O6	171.4(3)	O58–Mo18– O80	86.3(3)	O129–Mo25– O45	165.6(4)
O93–Mo3–O12	98.6(3)	O58–Mo18– O98	155.5(3)	O129–Mo25– O53	103.7(4)
O93–Mo3–O38	96.8(3)	O80–Mo18– O43	78.5(2)	O129–Mo25– O56	97.6(4)
O93–Mo3–O44	102.5(3)	O81–Mo18– O43	89.7(3)	O129–Mo25– O60	86.5(3)
O93–Mo3–O62	104.3(4)	O81–Mo18– O58	91.1(3)	O69–Mo26– O18	69.9(2)
O9–Mo4–O1	78.5(3)	O81–Mo18–	168.0(3)	O73–Mo26–	87.4(3)

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		O80		O18	
O9–Mo4–O83	81.5(3)	O81–Mo18– O98	93.8(3)	O73–Mo26– O69	156.3(3)
O41–Mo4–O1	85.2(3)	O98–Mo18– O43	72.0(3)	O73–Mo26– O79	89.3(3)
O41–Mo4–O9	161.6(3)	O98–Mo18– O80	84.0(3)	O79–Mo26– O18	70.2(3)
O41–Mo4–O83	87.8(3)	O148–Mo18– O43	168.9(3)	O79–Mo26– O69	77.0(3)
O59–Mo4–O1	85.9(3)	O148–Mo18– O58	99.8(4)	O88–Mo26– O18	86.2(3)
O59–Mo4–O9	92.4(3)	O148–Mo18– O80	91.4(3)	O88–Mo26– O69	89.5(3)
O59–Mo4–O41	94.9(3)	O148–Mo18– O81	100.6(3)	O88–Mo26– O73	95.9(3)
O59–Mo4–O83	167.2(3)	O148–Mo18– O98	102.8(4)	O88–Mo26– O79	155.6(3)
O83–Mo4–O1	81.8(3)	O28–Mo19– O32	84.7(3)	O144–Mo26– O18	162.6(3)
O97–Mo4–O1	171.0(3)	O28–Mo19– O42	150.2(3)	O144–Mo26– O69	96.3(4)
O97–Mo4–O9	94.7(3)	O28–Mo19– O78	99.5(3)	O144–Mo26– O73	104.5(4)
O97–Mo4–O41	100.5(3)	O28–Mo19– O86	85.6(3)	O144–Mo26– O79	96.9(4)
O97–Mo4–O59	100.5(3)	O42–Mo19– O32	72.6(3)	O144–Mo26– O88	104.8(4)
O97–Mo4–O83	91.3(3)	O42–Mo19– O86	73.0(3)	O10–Mo27– O23	76.0(2)
O19–Mo5–O13	78.3(3)	O78–Mo19– O32	74.6(3)	O34–Mo27– O10	81.6(3)
O19–Mo5–O62	82.1(3)	O78–Mo19– O42	92.9(3)	O34–Mo27– O23	81.2(3)
O52–Mo5–O13	86.3(3)	O78–Mo19– O86	156.6(3)	O96–Mo27– O10	79.6(3)
O52–Mo5–O19	93.2(3)	O86–Mo19– O32	83.3(3)	O96–Mo27– O23	79.0(3)
O52–Mo5–O58	95.4(3)	O127–Mo19– O28	105.0(4)	O96–Mo27– O34	155.4(3)
O52–Mo5–O62	167.9(3)	O127–Mo19– O32	170.3(3)	O130–Mo27– O10	165.2(3)
O58–Mo5–O13	84.9(3)	O127–Mo19– O42	98.5(3)	O130–Mo27– O23	89.4(3)
O58–Mo5–O19	160.6(3)	O127–Mo19–	102.5(4)	O130–Mo27–	94.1(4)

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		O78		O34	
O58–Mo5–O62	86.0(3)	O127–Mo19– O86	98.0(3)	O130–Mo27– O96	100.0(4)
O62–Mo5–O13	81.8(3)	O66–Mo20– O32	87.3(3)	O134–Mo27– O10	91.6(3)
O103–Mo5– O13	170.2(3)	O66–Mo20– O78	91.5(3)	O134–Mo27– O23	167.6(3)
O103–Mo5– O19	93.9(3)	O66–Mo20– O84	95.2(3)	O134–Mo27– O34	96.2(3)
O103–Mo5– O52	100.2(3)	O66–Mo20– O91	157.1(3)	O134–Mo27– O96	100.1(4)
O103–Mo5– O58	101.7(4)	O78–Mo20– O32	70.2(3)	O134–Mo27– O130	102.9(4)
O103–Mo5– O62	91.3(3)	O78–Mo20– O91	75.9(3)	O65–Mo28– O31	71.8(3)
O36–Mo6–O3	77.9(3)	O84–Mo20– O32	86.6(3)	O65–Mo28– O88	82.3(3)
O36–Mo6–O68	82.5(3)	O84–Mo20– O78	155.5(3)	O77–Mo28– O31	88.6(3)
O50–Mo6–O3	85.0(3)	O84–Mo20– O91	89.4(3)	O77–Mo28– O65	92.6(3)
O50–Mo6–O36	94.0(3)	O91–Mo20– O32	70.6(3)	O77–Mo28– O88	167.5(3)
O50–Mo6–O68	168.0(3)	O121–Mo20– O32	163.7(3)	O77–Mo28– O95	91.1(3)
O50–Mo6–O76	91.2(3)	O121–Mo20– O66	103.5(4)	O88–Mo28– O31	79.0(3)
O68–Mo6–O3	83.1(3)	O121–Mo20– O78	97.0(4)	O95–Mo28– O31	85.0(3)
O76–Mo6–O3	82.8(3)	O121–Mo20– O84	104.2(4)	O95–Mo28– O65	156.4(3)
O76–Mo6–O36	159.5(3)	O121–Mo20– O91	97.0(3)	O95–Mo28– O88	89.3(3)
O76–Mo6–O68	88.3(3)	O45–Mo21– O47	83.8(3)	O132–Mo28– O31	168.4(4)
O136–Mo6–O3	174.7(3)	O56–Mo21– O45	72.9(3)	O132–Mo28– O65	100.2(4)
O136–Mo6– O36	97.8(4)	O56–Mo21– O47	73.2(3)	O132–Mo28– O77	100.3(4)
O136–Mo6– O50	98.5(3)	O87–Mo21– O45	85.6(3)	O132–Mo28– O88	91.8(3)
O136–Mo6– O68	93.3(3)	O87–Mo21– O47	86.1(3)	O132–Mo28– O95	102.1(4)
O136–Mo6–	101.0(4)	O87–Mo21–	151.4(3)	O67–Mo29–	85.0(3)

O76		O56		O43	
O29–Mo7–O4	78.6(3)	O87–Mo21– O124	100.4(4)	O67–Mo29– O74	88.4(3)
O29–Mo7–O72	82.5(3)	O124–Mo21– O45	157.9(3)	O67–Mo29– O85	92.8(3)
O35–Mo7–O4	86.0(3)	O124–Mo21– O47	75.5(3)	O67–Mo29– O98	155.4(3)
O35–Mo7–O29	92.2(3)	O124–Mo21– O56	93.4(3)	O74–Mo29– O43	78.9(3)
O35–Mo7–O72	167.9(3)	O135–Mo21– O45	98.7(4)	O85–Mo29– O43	87.3(3)
O35–Mo7–O95	94.4(3)	O135–Mo21– O47	169.8(3)	O85–Mo29– O74	166.0(3)
O72–Mo7–O4	82.3(3)	O135–Mo21– O56	97.9(4)	O85–Mo29– O98	91.1(3)
O95–Mo7–O4	84.4(3)	O135–Mo21– O87	103.9(4)	O98–Mo29– O43	71.0(3)
O95–Mo7–O29	161.2(3)	O135–Mo21– O124	100.4(4)	O98–Mo29– O74	82.2(3)
O95–Mo7–O72	87.6(3)	O33–Mo22– O11	82.6(3)	O102–Mo29– O43	170.3(3)
O113–Mo7–O4	171.2(3)	O33–Mo22– O61	82.0(3)	O102–Mo29– O67	101.5(4)
O113–Mo7– O29	94.4(4)	O35–Mo22– O11	85.1(3)	O102–Mo29– O74	93.9(3)
O113–Mo7– O35	99.8(3)	O35–Mo22– O33	167.4(3)	O102–Mo29– O85	99.5(4)
O113–Mo7– O72	91.5(3)	O35–Mo22– O61	93.1(3)	O102–Mo29– O98	101.7(4)
O113–Mo7– O95	101.7(4)	O35–Mo22– O101	92.2(3)	O48–Mo30– O17	71.5(3)
O28–Mo8–O5	82.3(3)	O61–Mo22– O11	77.8(3)	O48–Mo30– O66	82.9(3)
O28–Mo8–O64	81.9(3)	O42–Mo15– O63	72.2(3)	O54–Mo30– O17	85.0(3)
O52–Mo8–O5	84.3(3)	O63–Mo15– O32	83.4(2)	O54–Mo30– O48	156.1(3)
O52–Mo8–O28	166.4(3)	O83–Mo15– O32	85.0(3)	O54–Mo30– O66	88.5(3)
O52–Mo8–O64	93.0(3)	O83–Mo15– O42	149.3(3)	O54–Mo30– O81	93.5(3)
O54–Mo8–O5	84.2(3)	O83–Mo15– O63	84.8(3)	O66–Mo30– O17	78.8(3)
O54–Mo8–O28	89.8(3)	O83–Mo15–	101.0(3)	O81–Mo30–	88.2(3)

		O91		O17	
O54-Mo8-O52	91.0(3)	O91-Mo15-O32	75.9(3)	O81-Mo30-O48	90.0(3)
O54-Mo8-O64	160.5(3)	O91-Mo15-O42	93.8(3)	O81-Mo30-O66	166.6(3)
O64-Mo8-O5	77.3(3)	O91-Mo15-O63	157.8(3)	O137-Mo30-O17	168.3(3)
O115-Mo8-O5	173.5(3)	O107-Mo15-O32	170.2(3)	O137-Mo30-O48	100.1(4)
O115-Mo8-O28	94.5(3)	O107-Mo15-O42	98.6(3)	O137-Mo30-O54	102.6(4)
O115-Mo8-O52	98.6(3)	O107-Mo15-O63	98.3(3)	O137-Mo30-O66	92.3(3)
O115-Mo8-O54	101.5(4)	O107-Mo15-O83	104.8(4)	O137-Mo30-O81	100.1(3)
O115-Mo8-O64	96.7(4)	O107-Mo15-O91	100.8(4)	O33-Mo31-O47	85.0(3)
O7-Mo9-O26	75.9(2)	O39-Mo16-O24	75.2(3)	O33-Mo31-O55	100.1(4)
O40-Mo9-O7	81.0(3)	O53-Mo16-O24	80.1(3)	O33-Mo31-O56	150.5(3)
O40-Mo9-O26	79.9(3)	O53-Mo16-O39	80.5(3)	O33-Mo31-O60	85.7(3)
O51-Mo9-O7	78.9(3)	O96-Mo16-O24	78.9(3)	O55-Mo31-O47	74.8(3)
O51-Mo9-O26	79.8(3)	O96-Mo16-O39	79.1(3)	O55-Mo31-O56	92.4(3)
O51-Mo9-O40	154.4(3)	O96-Mo16-O53	153.8(3)	O55-Mo31-O60	157.0(3)
O114-Mo9-O7	164.7(3)	O131-Mo16-O24	89.2(4)	O56-Mo31-O47	72.6(3)
O114-Mo9-O26	88.8(3)	O131-Mo16-O39	164.1(4)	O56-Mo31-O60	73.1(3)
O114-Mo9-O40	95.2(3)	O131-Mo16-O53	94.3(4)	O60-Mo31-O47	83.6(3)
O114-Mo9-O51	100.0(3)	O131-Mo16-O96	101.0(4)	O126-Mo31-O33	105.0(4)
O114-Mo9-O138	101.9(4)	O131-Mo16-O140	102.5(4)	O126-Mo31-O47	170.0(3)
O138-Mo9-O7	93.3(3)	O140-Mo16-O24	168.1(3)	O126-Mo31-O55	102.7(4)
O138-Mo9-O26	168.9(3)	O140-Mo16-O39	93.0(3)	O126-Mo31-O56	98.1(4)
O138-Mo9-	96.0(3)	O140-Mo16-	96.5(4)	O126-Mo31-	97.2(4)

O40		O53		O60	
O138–Mo9–O51	100.9(3)	O140–Mo16–O96	100.7(4)	O44–Mo32–O6	70.7(2)
O8–Mo10–O27	76.4(3)	O40–Mo17–O42	144.8(3)	O70–Mo32–O6	71.2(2)
O21–Mo10–O8	81.1(3)	O40–Mo17–O63	85.1(3)	O70–Mo32–O44	77.0(3)
O21–Mo10–O27	81.1(3)	O40–Mo17–O86	84.3(3)	O74–Mo32–O6	87.9(3)
O51–Mo10–O8	80.1(3)	O42–Mo17–O63	69.1(3)	O74–Mo32–O44	158.0(3)
O51–Mo10–O21	155.4(3)	O42–Mo17–O86	69.6(3)	O74–Mo32–O70	91.4(3)
O51–Mo10–O27	79.2(3)	O86–Mo17–O63	83.2(3)	O74–Mo32–O80	96.5(3)
O117–Mo10–O8	94.0(3)	O104–Mo17–O40	104.3(3)	O80–Mo32–O6	84.4(3)
O117–Mo10–O21	97.0(3)	O104–Mo17–O42	97.9(3)	O80–Mo32–O44	86.9(3)
O117–Mo10–O27	170.4(3)	O104–Mo17–O63	86.6(3)	O80–Mo32–O70	154.1(3)
O117–Mo10–O51	99.9(3)	O104–Mo17–O86	166.1(3)	O145–Mo32–O6	163.1(3)
O117–Mo10–O122	101.2(4)	O104–Mo17–O125	101.9(4)	O145–Mo32–O44	95.2(4)
O122–Mo10–O8	164.2(3)	O125–Mo17–O40	104.0(4)	O145–Mo32–O70	96.9(3)
O122–Mo10–O21	92.8(3)	O125–Mo17–O42	97.6(3)	O145–Mo32–O74	104.8(4)
O122–Mo10–O27	88.3(3)	O125–Mo17–O63	165.2(3)	O145–Mo32–O80	104.7(4)
O122–Mo10–O51	101.2(3)	O125–Mo17–O86	86.2(3)	O77–Mo33–O22	89.4(3)
O12–Mo11–O6	72.2(2)	O58–Mo18–O43	84.1(3)	O77–Mo33–O82	92.4(4)
O12–Mo11–O15	72.6(3)	O58–Mo18–O80	86.3(3)	O77–Mo33–O94	168.2(3)
O15–Mo11–O6	83.1(2)	O58–Mo18–O98	155.5(3)	O82–Mo33–O22	72.0(3)
O30–Mo11–O6	85.7(3)	O80–Mo18–O43	78.5(2)	O82–Mo33–O94	82.9(3)
O30–Mo11–O12	151.0(3)	O81–Mo18–O43	89.7(3)	O94–Mo33–O22	78.9(3)
O30–Mo11–	86.6(3)	O81–Mo18–	91.1(3)	O101–Mo33–	85.0(3)

O15		O58		O22	
O30–Mo11– O70	99.5(3)	O81–Mo18– O80	168.0(3)	O101–Mo33– O77	92.7(3)
O70–Mo11–O6	73.8(3)	O81–Mo18– O98	93.8(3)	O101–Mo33– O82	156.4(3)
O70–Mo11– O12	92.2(3)	O98–Mo18– O43	72.0(3)	O101–Mo33– O94	87.5(3)
O70–Mo11– O15	155.5(3)	O98–Mo18– O80	84.0(3)	O141–Mo33– O22	169.0(3)
O89–Mo11–O6	169.7(3)	O148–Mo18– O43	168.9(3)	O141–Mo33– O77	99.6(4)
O89–Mo11– O12	98.8(3)	O148–Mo18– O58	99.8(4)	O141–Mo33– O82	100.9(4)
O89–Mo11– O15	99.0(3)	O148–Mo18– O80	91.4(3)	O141–Mo33– O94	92.0(3)
O89–Mo11– O30	104.4(3)	O148–Mo18– O81	100.6(3)	O141–Mo33– O101	100.9(4)
O89–Mo11– O70	102.3(3)	O148–Mo18– O98	102.8(4)	O65–Mo34– O31	71.7(3)
O20–Mo12– O25	82.1(2)	O28–Mo19– O32	84.7(3)	O65–Mo34– O73	82.5(3)
O34–Mo12– O20	85.1(3)	O28–Mo19– O42	150.2(3)	O73–Mo34– O31	79.7(3)
O34–Mo12– O25	84.9(3)	O28–Mo19– O78	99.5(3)	O76–Mo34– O31	85.4(3)
O34–Mo12– O46	145.1(3)	O28–Mo19– O86	85.6(3)	O76–Mo34– O65	156.2(3)
O46–Mo12– O20	68.7(3)	O42–Mo19– O32	72.6(3)	O76–Mo34– O73	87.5(3)
O46–Mo12– O25	69.3(3)	O42–Mo19– O86	73.0(3)	O76–Mo34– O123	93.4(3)
O100–Mo12– O20	163.2(3)	O78–Mo19– O32	74.6(3)	O123–Mo34– O31	88.5(3)
O100–Mo12– O25	84.7(3)	O78–Mo19– O42	92.9(3)	O123–Mo34– O65	92.1(3)
O100–Mo12– O34	104.0(3)	O78–Mo19– O86	156.6(3)	O123–Mo34– O73	168.0(3)
O100–Mo12– O46	97.0(3)	O86–Mo19– O32	83.3(3)	O142–Mo34– O31	168.6(4)
O133–Mo12– O20	87.8(3)	O127–Mo19– O28	105.0(4)	O142–Mo34– O65	100.6(4)
O133–Mo12– O25	165.8(3)	O127–Mo19– O32	170.3(3)	O142–Mo34– O73	91.2(4)
O133–Mo12–	104.1(4)	O127–Mo19–	98.5(3)	O142–Mo34–	101.1(4)

O34		O42		O76	
O133–Mo12– O46	97.8(4)	O127–Mo19– O78	102.5(4)	O142–Mo34– O123	100.3(4)
O133–Mo12– O100	103.2(4)	O127–Mo19– O86	98.0(3)	O82–Mo35– O22	72.0(3)
O25–Mo13– O18	83.4(2)	O66–Mo20– O32	87.3(3)	O82–Mo35– O108	83.4(3)
O46–Mo13– O18	73.7(3)	O66–Mo20– O78	91.5(3)	O108–Mo35– O22	79.1(3)
O46–Mo13– O25	73.3(3)	O66–Mo20– O84	95.2(3)	O110–Mo35– O22	84.8(3)
O69–Mo13– O18	75.4(3)	O66–Mo20– O91	157.1(3)	O110–Mo35– O82	156.5(3)
O69–Mo13– O25	157.5(3)	O78–Mo20– O32	70.2(3)	O110–Mo35– O108	88.7(3)
O69–Mo13– O46	93.3(3)	O78–Mo20– O91	75.9(3)	O123–Mo35– O22	87.5(3)
O72–Mo13– O18	85.9(3)	O84–Mo20– O32	86.6(3)	O123–Mo35– O82	93.0(3)
O72–Mo13– O25	85.0(3)	O84–Mo20– O78	155.5(3)	O123–Mo35– O108	166.6(3)
O72–Mo13– O46	151.4(3)	O84–Mo20– O91	89.4(3)	O123–Mo35– O110	89.7(3)
O72–Mo13– O69	100.7(3)	O91–Mo20– O32	70.6(3)	O139–Mo35– O22	170.1(4)
O105–Mo13– O18	170.1(3)	O121–Mo20– O32	163.7(3)	O139–Mo35– O82	101.9(4)
O105–Mo13– O25	98.0(3)	O121–Mo20– O66	103.5(4)	O139–Mo35– O108	92.6(4)
O105–Mo13– O46	97.2(3)	O121–Mo20– O78	97.0(4)	O139–Mo35– O110	100.5(4)
O105–Mo13– O69	101.6(4)	O121–Mo20– O84	104.2(4)	O139–Mo35– O123	100.8(4)
O105–Mo13– O72	104.0(4)	O121–Mo20– O91	97.0(3)	O55–Mo36– O47	70.2(3)
O20–Mo14– O18	83.5(2)	O45–Mo21– O47	83.8(3)	O94–Mo36– O47	86.5(3)
O46–Mo14– O18	72.3(3)	O56–Mo21– O45	72.9(3)	O94–Mo36– O55	90.7(3)
O46–Mo14– O20	72.8(3)	O56–Mo21– O47	73.2(3)	O94–Mo36– O108	95.9(4)
O68–Mo14– O18	85.9(3)	O87–Mo21– O45	85.6(3)	O94–Mo36– O124	155.8(3)
O68–Mo14–	87.0(3)	O87–Mo21–	86.1(3)	O108–Mo36–	86.5(3)

O20		O47		O47	
O68–Mo14–O46	151.5(3)	O87–Mo21–O56	151.4(3)	O108–Mo36–O55	155.3(3)
O68–Mo14–O79	98.3(3)	O87–Mo21–O124	100.4(4)	O108–Mo36–O124	88.9(3)
O79–Mo14–O18	73.5(3)	O124–Mo21–O45	157.9(3)	O57–Cu1–O1W	90.6(4)
O79–Mo14–O20	155.9(3)	O124–Mo21–O47	75.5(3)	O57–Cu1–O2W	90.3(4)
O79–Mo14–O46	92.9(3)	O124–Mo21–O56	93.4(3)	O92–Cu1–O1W	88.5(4)
O106–Mo14–O18	169.6(3)	O135–Mo21–O45	98.7(4)	O92–Cu1–O2W	90.6(4)
O106–Mo14–O20	99.3(3)	O101–Mo22–O11	83.7(3)	O92–Cu1–O57	179.0(4)
O106–Mo14–O46	98.8(3)	O101–Mo22–O33	88.8(3)	N5–Cu2–N7	168.9(5)
O106–Mo14–O68	104.2(4)	O101–Mo22–O61	160.2(3)	N12–Cu3–N8	169.1(5)
O106–Mo14–O79	102.1(4)	O118–Mo22–O11	174.0(4)	N24–Cu4–N22	162.9(8)
O42–Mo15–O32	72.7(3)	O118–Mo22–O33	94.1(3)	N45–Cu5–N34	164.0(12)
O42–Mo15–O63	72.2(3)	O118–Mo22–O35	98.0(3)	N20–Cu6–N19	165.8(6)
O63–Mo15–O32	83.4(2)	O118–Mo22–O61	96.8(4)	N31–Cu7–N28	176.7(9)
O83–Mo15–O32	85.0(3)	O118–Mo22–O101	101.3(4)	N33–Cu8–N13	166.7(5)
O83–Mo15–O42	149.3(3)	O41–Mo23–O17	84.5(3)	N38–Cu9–N43	176.8(10)
O83–Mo15–O63	84.8(3)				

Table S4. The bond lengths (Å) in complex **2**.

Mo1–O27	2.232	Mo14–O43	2.442	Mo27–O125	1.885
Mo1–O28	2.226	Mo14–O56	1.822	Mo27–O127	1.707
Mo1–O39	1.896	Mo14–O85	1.681	Mo28–O9	2.218
Mo1–O46	2.029	Mo14–O107	2.043	Mo28–O15	1.898
Mo1–O91	1.695	Mo15–O24	2.299	Mo28–O36	2.042
Mo1–O143	1.705	Mo15–O103	1.696	Mo28–O69	1.675
Mo2–O10	2.25	Mo15–O107	2.05	Mo28–O110	2.031
Mo2–O90	1.699	Mo15–O117	1.84	Mo28–O111	1.88
Mo2–O93	1.694	Mo15–O122	2.332	Mo29–O11	2.258

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Mo2-O115	2.272	Mo15-O137	1.703	Mo29-O31	1.974
Mo2-O117	1.987	Mo16-O43	2.43	Mo29-O39	1.918
Mo2-O125	1.919	Mo16-O68	1.811	Mo29-O82	1.715
Mo3-O1	1.773	Mo16-O71	1.779	Mo29-O116	2.241
Mo3-O19	2.045	Mo16-O98	1.682	Mo29-O146	1.692
Mo3-O64	1.811	Mo16-O107	2.064	Mo30-O18	2.092
Mo3-O95	1.686	Mo16-O122	2.105	Mo30-O19	2.052
Mo3-O113	2.431	Mo17-O8	2.216	Mo30-O45	1.774
Mo3-O114	2.128	Mo17-O33	2.019	Mo30-O112	1.827
Mo4-O14	2.263	Mo17-O53	1.875	Mo30-O113	2.396
Mo4-O40	1.886	Mo17-O67	1.891	Mo30-O139	1.679
Mo4-O44	1.922	Mo17-O77	2.041	Mo31-O6	2.217
Mo4-O96	1.68	Mo17-O145	1.688	Mo31-O13	2.033
Mo4-O123	2.124	Mo18-O17	2.305	Mo31-O47	1.897
Mo4-O124	1.867	Mo18-O49	1.881	Mo31-O50	2.027
Mo5-O14	2.3	Mo18-O120	1.935	Mo31-O51	1.875
Mo5-O34	1.897	Mo18-O126	1.867	Mo31-O129	1.679
Mo5-O44	1.934	Mo18-O132	2.097	Mo32-O18	2.329
Mo5-O54	2.109	Mo18-O144	1.681	Mo32-O19	2.065
Mo5-O126	1.872	Mo19-O26	2.318	Mo32-O42	1.836
Mo5-O142	1.672	Mo19-O32	2.31	Mo32-O89	1.7
Mo6-O16	2.316	Mo19-O35	2.041	Mo32-O114	2.307
Mo6-O20	2.049	Mo19-O46	1.846	Mo32-O135	1.707
Mo6-O23	2.321	Mo19-O138	1.702	Mo33-O7	2.196
Mo6-O31	1.845	Mo19-O140	1.698	Mo33-O41	2.035
Mo6-O88	1.705	Mo20-O37	2.279	Mo33-O49	1.885
Mo6-O128	1.703	Mo20-O52	1.894	Mo33-O71	2.033
Mo7-O3	2.193	Mo20-O75	1.854	Mo33-O87	1.684
Mo7-O53	1.861	Mo20-O78	1.924	Mo33-O109	1.874
Mo7-O57	2.042	Mo20-O81	2.121	Mo34-O37	2.287
Mo7-O61	2.063	Mo20-O102	1.676	Mo34-O78	1.918
Mo7-O134	1.882	Mo21-O25	2.302	Mo34-O84	1.864
Mo7-O136	1.674	Mo21-O47	1.892	Mo34-O101	1.694
Mo8-O15	1.869	Mo21-O72	2.087	Mo34-O130	2.11
Mo8-O17	2.251	Mo21-O73	1.941	Mo34-O134	1.877
Mo8-O48	2.118	Mo21-O75	1.881	Mo35-O59	2.086
Mo8-O97	1.686	Mo21-O100	1.676	Mo35-O63	2.063
Mo8-O120	1.965	Mo22-O32	2.11	Mo35-O66	2.4
Mo8-O124	1.882	Mo22-O35	2.058	Mo35-O72	1.81
Mo9-O5	2.19	Mo22-O59	1.807	Mo35-O92	1.802
Mo9-O51	1.854	Mo22-O66	2.419	Mo35-O106	1.681
Mo9-O52	1.881	Mo22-O77	1.776	Mo36-O25	2.256
Mo9-O62	2.05	Mo22-O99	1.688	Mo36-O67	1.877
Mo9-O79	1.686	Mo23-O21	2.394	Mo36-O73	1.944

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Mo9–O121	2.019	Mo23–O58	2.073	Mo36–O84	1.881
Mo10–O54	1.778	Mo23–O74	2.084	Mo36–O92	2.081
Mo10–O64	2.117	Mo23–O81	1.803	Mo36–O105	1.681
Mo10–O76	1.701	Mo23–O130	1.776	Sr1–O2	2.721
Mo10–O112	2.084	Mo23–O141	1.69	Sr1–O4	2.662
Mo10–O113	2.392	Mo24–O43	2.364	Sr1–O7	2.682
Mo10–O123	1.778	Mo24–O48	1.805	Sr1–O9	2.673
Mo11–O16	2.124	Mo24–O56	2.1	Sr1–O10	2.564
Mo11–O20	2.064	Mo24–O68	2.057	Sr1–O22	2.603
Mo11–O21	2.437	Mo24–O104	1.689	Sr1–O108	2.556
Mo11–O62	1.789	Mo24–O132	1.788	Sr1–O115	2.582
Mo11–O74	1.806	Mo25–O1	2.052	Sr1–O125	2.804
Mo11–O86	1.68	Mo25–O4	2.218	Sr2–O3	2.67
Mo12–O26	2.102	Mo25–O12	2.022	Sr2–O5	2.673
Mo12–O35	2.057	Mo25–O40	1.875	Sr2–O6	2.664
Mo12–O50	1.785	Mo25–O111	1.847	Sr2–O8	2.677
Mo12–O63	1.809	Mo25–O133	1.676	Sr2–O11	2.548
Mo12–O66	2.412	Mo26–O2	2.192	Sr2–O27	2.581
Mo12–O94	1.678	Mo26–O29	2.042	Sr2–O28	2.583
Mo13–O20	2.053	Mo26–O34	1.885	Sr2–O39	2.783
Mo13–O21	2.394	Mo26–O45	2.039	Sr2–O116	2.639
Mo13–O23	2.095	Mo26–O109	1.856	Na1–O1W	2.381
Mo13–O58	1.821	Mo26–O119	1.692	Na1–O2W	2.401
Mo13–O61	1.768	Mo27–O22	2.244	Na1–O30	2.26
Mo13–O83	1.687	Mo27–O42	2.003	Na1–O118	2.261
Mo14–O24	2.107	Mo27–O80	1.708	Mo27–O125	1.885
Mo14–O36	1.771				

Table S5. The bond angles (°) in complex **2**.

O28–Mo1–O27	77.09	O85–Mo14–O56	99.3	O69–Mo28–O110	97.38
O39–Mo1–O27	79.54	O85–Mo14–O107	99.89	O69–Mo28–O111	98.62
O39–Mo1–O28	79.65	O107–Mo14–O24	74.08	O110–Mo28–O9	79.26
O39–Mo1–O46	155.54	O107–Mo14–O43	72.37	O110–Mo28–O36	82.41
O46–Mo1–O27	80.7	O24–Mo15–O122	82.37	O111–Mo28–O9	84.11
O46–Mo1–O28	82.01	O103–Mo15–O24	165.71	O111–Mo28–O15	92.69
O91–Mo1–O27	166.53	O103–Mo15–O107	97.44	O111–Mo28–O36	166.97

O91-Mo1-O28	89.7	O103-Mo15-O117	103.23	O111-Mo28-O110	93.22
O91-Mo1-O39	100.91	O103-Mo15-O122	86.83	O31-Mo29-O11	81.78
O91-Mo1-O46	95.01	O103-Mo15-O137	102.86	O31-Mo29-O116	81.25
O91-Mo1-O143	102.04	O107-Mo15-O24	69.91	O39-Mo29-O11	76.55
O143-Mo1-O27	91.03	O107-Mo15-O122	68.61	O39-Mo29-O31	153.57
O143-Mo1-O28	167.87	O117-Mo15-O24	85.19	O39-Mo29-O116	79.44
O143-Mo1-O39	100.8	O117-Mo15-O107	145.45	O82-Mo29-O11	90.54
O143-Mo1-O46	93.81	O117-Mo15-O122	85.09	O82-Mo29-O31	95.7
O10-Mo2-O115	76.01	O137-Mo15-O24	85.63	O82-Mo29-O39	99.43
O90-Mo2-O10	91.63	O137-Mo15-O107	96.4	O82-Mo29-O116	167.94
O90-Mo2-O115	167.59	O137-Mo15-O117	105.44	O116-Mo29-O11	77.5
O90-Mo2-O117	97.06	O137-Mo15-O122	163.33	O146-Mo29-O11	166.77
O90-Mo2-O125	99.51	O68-Mo16-O43	74.86	O146-Mo29-O31	99.03
O93-Mo2-O10	165.63	O68-Mo16-O107	91.25	O146-Mo29-O39	98.69
O93-Mo2-O90	102.74	O68-Mo16-O122	155.05	O146-Mo29-O82	102.48
O93-Mo2-O115	89.64	O71-Mo16-O43	84.57	O146-Mo29-O116	89.54
O93-Mo2-O117	96.79	O71-Mo16-O68	99.48	O18-Mo30-O113	83.66
O93-Mo2-O125	99.66	O71-Mo16-O107	151.02	O19-Mo30-O18	73.86
O117-Mo2-O10	80.75	O71-Mo16-O122	86.87	O19-Mo30-O113	73.39
O117-Mo2-O115	82.16	O98-Mo16-O43	171.68	O45-Mo30-O18	87.15
O125-Mo2-O10	78.12	O98-Mo16-O68	102.95	O45-Mo30-O19	152.8
O125-Mo2-O115	77.19	O98-Mo16-O71	103.74	O45-Mo30-O112	99.33

O125–Mo2– O117	153.39	O98–Mo16– O107	99.88	O45–Mo30– O113	85.52
O1–Mo3– O19	149.85	O98–Mo16– O122	98.84	O112–Mo30– O18	156.64
O1–Mo3– O64	100.33	O107–Mo16– O43	72.31	O112–Mo30– O19	91.56
O1–Mo3– O113	84.3	O107–Mo16– O122	73.02	O112–Mo30– O113	74.59
O1–Mo3– O114	85.74	O122–Mo16– O43	81.83	O139–Mo30– O18	98.98
O19–Mo3– O113	72.73	O33–Mo17– O8	79.17	O139–Mo30– O19	97.92
O19–Mo3– O114	72.87	O33–Mo17– O77	82.49	O139–Mo30– O45	104.25
O64–Mo3– O19	92.54	O53–Mo17– O8	84.62	O139–Mo30– O112	101.07
O64–Mo3– O113	75.19	O53–Mo17– O33	93.82	O139–Mo30– O113	169.94
O64–Mo3– O114	157.41	O53–Mo17– O67	92.19	O13–Mo31– O6	78.94
O95–Mo3– O1	104.55	O53–Mo17– O77	167.65	O47–Mo31– O6	84.43
O95–Mo3– O19	99.4	O67–Mo17– O8	82.84	O47–Mo31– O13	161.65
O95–Mo3– O64	101.35	O67–Mo17– O33	160.39	O47–Mo31– O50	87.42
O95–Mo3– O113	171.03	O67–Mo17– O77	87.69	O50–Mo31– O6	82.73
O95–Mo3– O114	98.06	O77–Mo17– O8	83.11	O50–Mo31– O13	82.84
O114–Mo3– O113	83.89	O145–Mo17– O8	176.06	O51–Mo31– O6	84.11
O40–Mo4– O14	84.95	O145–Mo17– O33	97.87	O51–Mo31– O13	93.09
O40–Mo4– O44	157.08	O145–Mo17– O53	98.23	O51–Mo31– O47	92.88
O40–Mo4– O123	87.6	O145–Mo17– O67	99.71	O51–Mo31– O50	166.74
O44–Mo4– O14	72.63	O145–Mo17– O77	93.96	O129–Mo31– O6	173.87
O44–Mo4– O123	83.43	O49–Mo18– O17	84.77	O129–Mo31– O13	95.69
O96–Mo4– O14	167.82	O49–Mo18– O120	155.89	O129–Mo31– O47	100.45

O96–Mo4– O40	100.99	O49–Mo18– O132	86.98	O129–Mo31– O50	93.72
O96–Mo4– O44	100.21	O120–Mo18– O17	71.51	O129–Mo31– O51	99.25
O96–Mo4– O123	91.02	O120–Mo18– O132	84.06	O19–Mo32– O18	68.74
O96–Mo4– O124	101.32	O126–Mo18– O17	87.76	O19–Mo32– O114	68.85
O123–Mo4– O14	78.52	O126–Mo18– O49	91.5	O42–Mo32– O18	83.29
O124–Mo4– O14	89.03	O126–Mo18– O120	91.76	O42–Mo32– O19	144.67
O124–Mo4– O40	91.66	O126–Mo18– O132	165.81	O42–Mo32– O114	86.56
O124–Mo4– O44	92.63	O132–Mo18– O17	78.05	O89–Mo32– O18	87.97
O124–Mo4– O123	167.55	O144–Mo18– O17	168.86	O89–Mo32– O19	96.36
O34–Mo5– O14	84.56	O144–Mo18– O49	101.72	O89–Mo32– O42	104.01
O34–Mo5– O44	155.56	O144–Mo18– O120	101.08	O89–Mo32– O114	164.21
O34–Mo5– O54	86.67	O144–Mo18– O126	100.98	O89–Mo32– O135	102.61
O44–Mo5– O14	71.56	O144–Mo18– O132	93.14	O114–Mo32– O18	81.57
O44–Mo5– O54	83.67	O32–Mo19– O26	82.31	O135–Mo32– O18	164.95
O54–Mo5– O14	78.63	O35–Mo19– O26	69	O135–Mo32– O19	99.11
O126–Mo5– O14	87.59	O35–Mo19– O32	69.8	O135–Mo32– O42	104.1
O126–Mo5– O34	91.64	O46–Mo19– O26	84.81	O135–Mo32– O114	85.76
O126–Mo5– O44	92.45	O46–Mo19– O32	84.74	O41–Mo33– O7	78.34
O126–Mo5– O54	166.21	O46–Mo19– O35	145.19	O49–Mo33– O7	84.58
O142–Mo5– O14	169.19	O138–Mo19– O26	166.24	O49–Mo33– O41	161.27
O142–Mo5– O34	102.72	O138–Mo19– O32	87.46	O49–Mo33– O71	88.5
O142–Mo5– O44	100.26	O138–Mo19– O35	98.85	O71–Mo33– O7	82.71

O142–Mo5– O54	93.67	O138–Mo19– O46	103.45	O71–Mo33– O41	81.82
O142–Mo5– O126	100.05	O140–Mo19– O26	86.31	O87–Mo33– O7	172.75
O16–Mo6– O23	82.33	O140–Mo19– O32	165.81	O87–Mo33– O41	95.37
O20–Mo6– O16	69.13	O140–Mo19– O35	98.21	O87–Mo33– O49	101.11
O20–Mo6– O23	69.22	O140–Mo19– O46	102.69	O87–Mo33– O71	92.88
O31–Mo6– O16	83.45	O140–Mo19– O138	102.27	O87–Mo33– O109	98.24
O31–Mo6– O20	144.71	O52–Mo20– O37	83.81	O109–Mo33– O7	85.89
O31–Mo6– O23	85.92	O52–Mo20– O78	155.28	O109–Mo33– O41	93.69
O88–Mo6– O16	165.05	O52–Mo20– O81	87.27	O109–Mo33– O49	92.68
O88–Mo6– O20	98.99	O75–Mo20– O37	88.46	O109–Mo33– O71	168.37
O88–Mo6– O23	84.95	O75–Mo20– O52	91.62	O78–Mo34– O37	71.83
O88–Mo6– O31	103.46	O75–Mo20– O78	92.3	O78–Mo34– O130	83.3
O128–Mo6– O16	88.41	O75–Mo20– O81	167.58	O84–Mo34– O37	88.12
O128–Mo6– O20	97.29	O78–Mo20– O37	71.91	O84–Mo34– O78	92.41
O128–Mo6– O23	165.67	O78–Mo20– O81	83.72	O84–Mo34– O130	166.62
O128–Mo6– O31	103.92	O81–Mo20– O37	79.13	O84–Mo34– O134	91.27
O128–Mo6– O88	102.47	O102–Mo20– O37	168.93	O101–Mo34– O37	169.44
O53–Mo7– O3	86.26	O102–Mo20– O52	100.95	O101–Mo34– O78	101.06
O53–Mo7– O57	92.78	O102–Mo20– O75	101.3	O101–Mo34– O84	100.18
O53–Mo7– O61	167.63	O102–Mo20– O78	102.19	O101–Mo34– O130	93.1
O53–Mo7– O134	94.26	O102–Mo20– O81	91.04	O101–Mo34– O134	101.63
O57–Mo7– O3	78.06	O47–Mo21– O25	85	O130–Mo34– O37	78.5

O57–Mo7– O61	81.54	O47–Mo21– O72	86.87	O134–Mo34– O37	84.57
O61–Mo7– O3	81.83	O47–Mo21– O73	156.23	O134–Mo34– O78	155.97
O134–Mo7– O3	84.57	O72–Mo21– O25	78.79	O134–Mo34– O130	87.69
O134–Mo7– O57	160.78	O73–Mo21– O25	71.64	O59–Mo35– O66	70.98
O134–Mo7– O61	87.94	O73–Mo21– O72	84.37	O63–Mo35– O59	76.88
O136–Mo7– O3	170.98	O75–Mo21– O25	87.43	O63–Mo35– O66	71.88
O136–Mo7– O53	100	O75–Mo21– O47	91.51	O72–Mo35– O59	156.52
O136–Mo7– O57	95.03	O75–Mo21– O72	166.21	O72–Mo35– O63	89.45
O136–Mo7– O61	91.49	O75–Mo21– O73	91.79	O72–Mo35– O66	86.75
O136–Mo7– O134	101.31	O100–Mo21– O25	170.13	O92–Mo35– O59	89.35
O15–Mo8– O17	85.67	O100–Mo21– O47	101.3	O92–Mo35– O63	156.31
O15–Mo8– O48	89.2	O100–Mo21– O72	93.85	O92–Mo35– O66	85.51
O15–Mo8– O120	157.5	O100–Mo21– O73	101.31	O92–Mo35– O72	96.41
O15–Mo8– O124	92.33	O100–Mo21– O75	99.89	O106–Mo35– O59	96.38
O48–Mo8– O17	79.75	O32–Mo22– O66	84.84	O106–Mo35– O63	96.42
O97–Mo8– O15	103.12	O35–Mo22– O32	73.68	O106–Mo35– O66	164.17
O97–Mo8– O17	167.91	O35–Mo22– O66	72.64	O106–Mo35– O72	104.14
O97–Mo8– O48	91.94	O59–Mo22– O32	157.85	O106–Mo35– O92	104.29
O97–Mo8– O120	98.17	O59–Mo22– O35	91.37	O67–Mo36– O25	85.71
O97–Mo8– O124	99.11	O59–Mo22– O66	74.96	O67–Mo36– O73	157.95
O120–Mo8– O17	72.25	O77–Mo22– O32	86.55	O67–Mo36– O84	92.23
O120–Mo8– O48	82.82	O77–Mo22– O35	151.43	O67–Mo36– O92	88.43

O124–Mo8– O17	88.68	O77–Mo22– O59	100.6	O73–Mo36– O25	72.65
O124–Mo8– O48	168.18	O77–Mo22– O66	85.45	O73–Mo36– O92	83.48
O124–Mo8– O120	91.43	O99–Mo22– O32	98.28	O84–Mo36– O25	88.24
O51–Mo9– O5	85.87	O99–Mo22– O35	98.19	O84–Mo36– O73	91.34
O51–Mo9– O52	93.58	O99–Mo22– O59	100.01	O84–Mo36– O92	167.4
O51–Mo9– O62	168.89	O99–Mo22– O66	169.18	O92–Mo36– O25	79.25
O51–Mo9– O121	93.78	O99–Mo22– O77	105.02	O105–Mo36– O25	169.32
O52–Mo9– O5	84.02	O58–Mo23– O21	71.26	O105–Mo36– O67	101.89
O52–Mo9– O62	87.55	O58–Mo23– O74	76.56	O105–Mo36– O73	99.04
O52–Mo9– O121	161.28	O74–Mo23– O21	71.17	O105–Mo36– O84	98.84
O62–Mo9– O5	83.26	O81–Mo23– O21	87.02	O105–Mo36– O92	93.33
O79–Mo9– O5	173.01	O81–Mo23– O58	156.46	O2–Sr1– O125	131.74
O79–Mo9– O51	98.26	O81–Mo23– O74	88.12	O4–Sr1–O2	53.97
O79–Mo9– O52	101.27	O130–Mo23– O21	86.8	O4–Sr1–O7	95.99
O79–Mo9– O62	92.34	O130–Mo23– O58	90.79	O4–Sr1–O9	73.12
O79–Mo9– O121	94.67	O130–Mo23– O74	157.11	O4–Sr1– O125	131.75
O121–Mo9– O5	79.37	O130–Mo23– O81	97.12	O7–Sr1–O2	71.62
O121–Mo9– O62	82.01	O141–Mo23– O21	161.68	O7–Sr1– O125	132.25
O54–Mo10– O64	157.44	O141–Mo23– O58	94.46	O9–Sr1–O2	96.74
O54–Mo10– O112	91.04	O141–Mo23– O74	94.78	O9–Sr1–O7	54.27
O54–Mo10– O113	87.46	O141–Mo23– O81	104.68	O9–Sr1– O125	131.51
O64–Mo10– O113	71.2	O141–Mo23– O130	105.3	O10–Sr1–O2	169.54

O76–Mo10– O54	105.3	O48–Mo24– O43	87.46	O10–Sr1–O4	120.26
O76–Mo10– O64	93.85	O48–Mo24– O56	88.89	O10–Sr1–O7	101.87
O76–Mo10– O112	94.79	O48–Mo24– O68	158.15	O10–Sr1–O9	72.82
O76–Mo10– O113	161.05	O56–Mo24– O43	71.52	O10–Sr1– O22	117.77
O76–Mo10– O123	105.52	O68–Mo24– O43	72.43	O10–Sr1– O115	65.5
O112–Mo10– O64	75.31	O68–Mo24– O56	76.87	O10–Sr1– O125	58.7
O112–Mo10– O113	70.61	O104–Mo24– O43	162.64	O22–Sr1–O2	72.69
O123–Mo10– O54	97.08	O104–Mo24– O48	102.7	O22–Sr1–O4	102.09
O123–Mo10– O64	88.97	O104–Mo24– O56	94.38	O22–Sr1–O7	117.6
O123–Mo10– O112	155.16	O104–Mo24– O68	94.94	O22–Sr1–O9	168.96
O123–Mo10– O113	86.29	O104–Mo24– O132	105.03	O22–Sr1– O125	59.11
O16–Mo11– O21	82.94	O132–Mo24– O43	87.53	O108–Sr1– O2	101.35
O20–Mo11– O16	72.82	O132–Mo24– O48	96.23	O108–Sr1– O4	73.57
O20–Mo11– O21	72.28	O132–Mo24– O56	158.23	O108–Sr1– O7	169.57
O62–Mo11– O16	86.17	O132–Mo24– O68	91.48	O108–Sr1– O9	120.69
O62–Mo11– O20	150.93	O1–Mo25– O4	81.87	O108–Sr1– O10	83.89
O62–Mo11– O21	85.64	O12–Mo25– O1	82.31	O108–Sr1– O22	65.87
O62–Mo11– O74	99.68	O12–Mo25– O4	77.88	O108–Sr1– O115	116.4
O74–Mo11– O16	156.15	O40–Mo25– O1	87.67	O108–Sr1– O125	58.18
O74–Mo11– O20	92.56	O40–Mo25– O4	84.11	O115–Sr1– O2	118.8
O74–Mo11– O21	74.55	O40–Mo25– O12	160.43	O115–Sr1– O4	169.69
O86–Mo11– O16	99.16	O111–Mo25– O1	167.16	O115–Sr1– O7	74.02

O86–Mo11– O20	98.98	O111–Mo25– O4	85.57	O115–Sr1– O9	102.15
O86–Mo11– O21	170.09	O111–Mo25– O12	92.51	O115–Sr1– O22	80.88
O86–Mo11– O62	104.12	O111–Mo25– O40	93.68	O115–Sr1– O125	58.25
O86–Mo11– O74	101.73	O133–Mo25– O1	92.68	O3–Sr2–O5	54.5
O26–Mo12– O66	81.62	O133–Mo25– O4	172.11	O3–Sr2–O8	73
O35–Mo12– O26	73.17	O133–Mo25– O12	95.79	O3–Sr2–O39	130.79
O35–Mo12– O66	72.81	O133–Mo25– O40	101.45	O5–Sr2–O8	97.86
O50–Mo12– O26	87.03	O133–Mo25– O111	99.54	O5–Sr2–O39	131.27
O50–Mo12– O35	151.87	O29–Mo26– O2	78.36	O6–Sr2–O3	96.98
O50–Mo12– O63	98.61	O34–Mo26– O2	84.69	O6–Sr2–O5	73.22
O50–Mo12– O66	84.9	O34–Mo26– O29	161.49	O6–Sr2–O8	54.56
O63–Mo12– O26	155.96	O34–Mo26– O45	88.38	O6–Sr2–O39	132.23
O63–Mo12– O35	92.39	O45–Mo26– O2	82.62	O8–Sr2–O39	130.86
O63–Mo12– O66	75.69	O45–Mo26– O29	82.18	O11–Sr2–O3	72.58
O94–Mo12– O26	98.5	O109–Mo26– O2	85.09	O11–Sr2–O5	100.21
O94–Mo12– O35	99.13	O109–Mo26– O29	92.16	O11–Sr2–O6	169.55
O94–Mo12– O50	103.5	O109–Mo26– O34	93.75	O11–Sr2–O8	119.88
O94–Mo12– O63	102.78	O109–Mo26– O45	167.28	O11–Sr2– O27	84.63
O94–Mo12– O66	171.6	O119–Mo26– O2	172.11	O11–Sr2– O28	117.28
O20–Mo13– O21	73.4	O119–Mo26– O29	94.98	O11–Sr2– O39	58.21
O20–Mo13– O23	73.84	O119–Mo26– O34	101.3	O11–Sr2– O116	65.74
O23–Mo13– O21	84.05	O119–Mo26– O45	92.34	O27–Sr2–O3	119.37

O58–Mo13– O20	91.96	O119–Mo26– O109	99.52	O27–Sr2–O5	169.53
O58–Mo13– O21	75.36	O22–Mo27– O108	76.86	O27–Sr2–O6	100.58
O58–Mo13– O23	157.74	O42–Mo27– O22	80.96	O27–Sr2–O8	71.72
O61–Mo13– O20	151.43	O42–Mo27– O108	80.33	O27–Sr2– O28	65.08
O61–Mo13– O21	84.6	O80–Mo27– O22	90.14	O27–Sr2– O39	59.14
O61–Mo13– O23	86.17	O80–Mo27– O42	97.64	O27–Sr2– O116	118
O61–Mo13– O58	100.01	O80–Mo27– O108	167	O28–Sr2–O3	170.05
O83–Mo13– O20	98.49	O80–Mo27– O125	100.8	O28–Sr2–O5	119.52
O83–Mo13– O21	170.51	O125–Mo27– O22	80.18	O28–Sr2–O6	73.17
O83–Mo13– O23	98.61	O125–Mo27– O42	153.53	O28–Sr2–O8	101.48
O83–Mo13– O58	100.42	O125–Mo27– O108	77.42	O28–Sr2– O39	59.1
O83–Mo13– O61	104.62	O127–Mo27– O22	167.59	O28–Sr2– O116	81.64
O24–Mo14– O43	85.28	O127–Mo27– O42	94.92	O116–Sr2– O3	102.44
O36–Mo14– O24	86.1	O127–Mo27– O80	102.04	O116–Sr2– O5	72.46
O36–Mo14– O43	85.03	O127–Mo27– O108	90.93	O116–Sr2– O6	118.38
O36–Mo14– O56	100.13	O127–Mo27– O125	99.57	O116–Sr2– O8	169.96
O36–Mo14– O107	150.79	O15–Mo28– O9	83.11	O116–Sr2– O39	58.92
O56–Mo14– O24	157.77	O15–Mo28– O36	87.77	O1W–Na1– O2W	178.43
O56–Mo14– O43	74.14	O15–Mo28– O110	160.7	O30–Na1– O1W	90.02
O56–Mo14– O107	91.41	O36–Mo28– O9	83.02	O30–Na1– O2W	89.44
O85–Mo14– O24	99.72	O69–Mo28– O9	175.82	O30–Na1– O118	176.04
O85–Mo14– O36	104.52	O69–Mo28– O15	99.87	O118–Na1– O1W	86.23

O85–Mo14– O43	169.41	O69–Mo28– O36	94.12	O118–Na1– O2W	94.28
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Table S6. Selected hydrogen bonding geometry (Å, °) for complex **1**.

D–H···A	D–H	H···A	D···A	D–H···A
N2–H2A···O49	0.86	1.84	2.619	151
N3–H3A···O125	0.86	1.91	2.753	165
N21–H21···O97	0.86	2.26	2.978	141
N23–H23···O105	0.86	2.12	2.897	149
N32–H32···O93	0.86	2.25	3.050	153
N41–H41A···O62	0.86	2.37	3.045	135
N42–H42A···O65	0.86	1.91	2.750	165
N46– H46A···O119	0.86	2.36	3.08	142

Table S7. Selected hydrogen bonding geometry (Å, °) for complex **2**.

D–H···A	D–H	H···A	D···A	D–H···A
N2–H2A···O131	0.86	1.81	2.670	176
N12–H12···O99	0.86	2.30	3.059	148
N1–H1···O55	0.86	1.83	2.658	162
N4–H4···O56	0.86	1.95	2.805	173
N23–H23A···O65	0.86	1.75	2.611	175
N24–H24A···O79	0.86	2.09	2.703	128
N28– H28A···O145	0.86	2.19	2.909	142
N27–H27A···O80	0.86	2.02	2.824	154

Table S8. BVS values for Mo atoms in complex **1**

Atom	Mo <sup>V</sup>	Mo <sup>VI</sup>	Average
Mo1	5.92	6.03	5.98
Mo2	5.45	5.84	5.65
Mo3	5.91	6.02	5.97
Mo4	5.69	5.80	5.74
Mo5	5.75	5.86	5.81
Mo6	5.78	5.89	5.83
Mo7	5.76	5.87	5.81
Mo8	5.66	5.76	5.71
Mo9	5.92	6.04	5.98
Mo10	5.98	6.09	6.03
Mo11	5.92	6.03	5.97
Mo12	5.87	5.98	5.92
Mo13	5.90	6.02	5.96

Mo14	5.90	6.01	5.96
Mo15	5.97	6.08	6.03
Mo16	5.92	6.03	5.98
Mo17	5.95	6.06	6.00
Mo18	5.69	5.79	5.74
Mo19	5.86	5.97	5.91
Mo20	5.87	5.99	5.93
Mo21	5.92	6.03	5.98
Mo22	5.63	5.74	5.69
Mo23	5.97	6.09	6.03
Mo24	5.69	5.80	5.75
Mo25	5.97	6.08	6.03
Mo26	5.99	6.10	6.04
Mo27	6.03	6.14	6.09
Mo28	5.75	5.86	5.81
Mo29	5.86	5.97	5.91
Mo30	5.58	5.68	5.63
Mo31	5.83	5.94	5.88
Mo32	5.95	6.06	6.01
Mo33	5.75	5.86	5.81
Mo34	5.65	5.75	5.70
Mo35	5.78	5.89	5.84
Mo36	5.92	6.03	5.98
	5.83	5.95	5.89

Table S9. BVS values for Mo atoms in complex 2

Atom	MoV	MoVI	Average
Mo1	5.63	6.09	5.86
Mo2	5.62	6.08	5.85
Mo3	5.58	6.03	5.80
Mo4	5.47	5.92	5.70
Mo5	5.43	5.87	5.65
Mo6	5.53	5.98	5.76
Mo7	5.45	5.89	5.67
Mo8	5.37	5.81	5.59
Mo9	5.48	5.93	5.70
Mo10	5.58	6.04	5.81
Mo11	5.53	5.99	5.76
Mo12	5.61	6.06	5.83
Mo13	5.62	6.07	5.84
Mo14	5.60	6.05	5.83
Mo15	5.59	6.05	5.82
Mo16	5.58	6.03	5.80
Mo17	5.37	5.81	5.59

Mo18	5.45	5.90	5.67
Mo19	5.59	6.04	5.81
Mo20	5.49	5.94	5.71
Mo21	5.41	5.85	5.63
Mo22	5.58	6.04	5.81
Mo23	5.62	6.07	5.84
Mo24	5.59	6.05	5.82
Mo25	5.52	5.97	5.75
Mo26	5.41	5.85	5.63
Mo27	5.58	6.04	5.81
Mo28	5.38	5.81	5.59
Mo29	5.61	6.07	5.84
Mo30	5.62	6.07	5.85
Mo31	5.40	5.84	5.62
Mo32	5.54	5.99	5.76
Mo33	5.42	5.86	5.64
Mo34	5.45	5.89	5.67
Mo35	5.55	6.01	5.78
Mo36	5.47	5.92	5.70
	5.52	5.97	5.74

Table S10. BVS values for Cu atoms in complex **1**

Atom	BVS	Atom	BVS	Atom	BVS
Cu1	1.85	Cu4	1.01	Cu7	1.01
Cu2	1.07	Cu5	1.01	Cu8	1.01
Cu3	1.10	Cu6	0.94	Cu9	0.96

Table S11. The influence of solvents on the catalytic reaction of BA. <sup>a</sup>

Entry	Solvent	Conv.of BA(%)	Sel. of BAD (%)	Sel. of BZA (%)
1	Diox	31.4	80.9	19.1
2	CYH	67.9	44.1	55.9
3	CH <sub>3</sub> CN	70.9	31.0	69.0
4	EtOH	38.3	68.3	31.7
5	EtOAc	43.0	62.5	37.5

<sup>a</sup> Reaction conditions: 0.5 mmol of BA, catalyst (0.8  $\mu$ mol), TBHP (1.5 mmol), CH<sub>3</sub>CN (1.0 mL), 70 °C, 6 h.

Table S12. The influence of catalyst dosage on the catalytic reaction of BA. <sup>a</sup>

Entry	Catalyst ( $\mu$ mol)	Conv. of BA(%)	Sel. of BAD (%)	Sel. of BZA (%)
1	0.6	88.7	18.6	81.4
2	0.8	94.0	11.4	88.6
3	1.0	96.5	7.4	92.6
4	1.2	98.5	3.3	96.7
5	1.4	99.2	1.8	98.2

6	1.6	99.6	1.8	98.2
7	1.8	99.6	1.3	98.7
8	2.0	99.5	1.4	98.6

<sup>a</sup> Reaction conditions: 0.5 mmol of BA, TBHP (2 mmol), CH<sub>3</sub>CN (1.0 mL), 75 °C, 8 h.

Table S13. The influence of TBHP dosage on the catalytic reaction of BA. <sup>a</sup>

Entry	TBHP (mmol)	Conv. of BA(%)	Sel. of BAD (%)	Sel. of BZA (%)
1	1	91.0	17.8	82.2
2	1.5	96.5	8.2	91.8
3	2	99.3	1.4	98.6
4	2.5	98.6	3.3	96.7
5	3	98.4	2.1	97.9

<sup>a</sup> Reaction conditions: 0.5 mmol of BA, catalyst (1.4 μmol), CH<sub>3</sub>CN (1.0 mL), 75 °C, 8 h.

Table S14. The influence of temperature on the catalytic reaction of BA. <sup>a</sup>

Entry	Temperature (°C)	Conv. of BA(%)	Sel. of BAD (%)	Sel. of BZA (%)
1	60	69.3	40.3	59.7
2	65	81.8	25.4	74.5
3	70	95.8	7.8	92.2
4	75	99.4	1.7	98.3
5	80	99.3	1.8	98.2

<sup>a</sup> Reaction conditions: 0.5 mmol of BA, Catalyst (1.4 μmol), TBHP (2 mmol), CH<sub>3</sub>CN (1.0 mL), 8 h.

Table S15. Catalytic performance of various POM-based catalysts for the oxidation of benzyl alcohol.

Catalyst	n <sub>substrate</sub> (mmol)	T (°C)	Oxidant	Time (h)	Conv. [%] <sup>a</sup>	Sel. [%] <sup>b</sup>	Ref.
Cu <sub>9</sub> [P <sub>6</sub> Mo <sub>18</sub> ] <sub>2</sub>	0.5	75	TBHP	8	99.5	98.4	This work
Cu <sub>9</sub> [P <sub>6</sub> Mo <sub>18</sub> ] <sub>2</sub>	5	75	TBHP	8	99.0	99.0	This work
Na[P <sub>6</sub> Mo <sub>18</sub> ] <sub>2</sub>	0.5	75	TBHP	8	67.0	41.2	This work
Cu <sub>3</sub> [Co <sub>2</sub> Mo <sub>10</sub> ]	0.25	75	TBHP	10	99.4	98.8	[3]
Cu <sub>2</sub> [Co <sub>2</sub> Mo <sub>10</sub> ]	0.25	75	TBHP	10	100	98.0	[4]
CuV <sub>2</sub>	0.25	120	H <sub>2</sub> O <sub>2</sub>	8	98.5	100 <sup>c</sup>	[5]
Cu <sub>12</sub> [P <sub>2</sub> Mo <sub>18</sub> ] <sub>2</sub>	0.5	70	TBHP	9	100	99.47	[6]

$\text{Cu}_{12}[\text{P}_2\text{Mo}_{18}]_2$	5	70	TBHP	9	99.6	98.2	[6]
$\text{Cu}_2\text{Mo}_8$	1.1	75	TBHP	24	85	70	[7]
PMo/DAIL/MIL-101(Cr)	1	100	TBHP	6	56	99 <sup>c</sup>	[8]
$\text{NH}_2\text{MIL88B(Fe)-}$	1	100	TBHP	8	87	99 <sup>c</sup>	[9]
$\text{H}_3\text{PMo}_{12}\text{O}_{40}$	1	100	TBHP	8	87	99 <sup>c</sup>	[9]
$\text{MnMo}_8$	4	80	$\text{H}_2\text{O}_2$	8	97	99 <sup>c</sup>	[10]

[a] Conversion of benzyl alcohol, [b] Selectivity of benzoic acid, [c] Selectivity of benzaldehyde.

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