Supporting Information

Development of a Uricase-Free Colorimetric Biosensor for Uric Acid Based on PPy-Coated Polyoxometalate-Encapsulated Fourfold Helical Metal–Organic Frameworks

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Section 1. Supplementary Figures and Tables

Table S1. Comparison of the advantages and disadvantages of some reported assay systems for UA detection.

Assay system	Advantages	Disadvantages	Ref.
Cu^{2+} (with uricase)	Sensitive and rapid	Unstable and unrepeatable	[1]
g-C_3N_4 (with uricase)	Sensitive and rapid	Unstable and unrepeatable	[2]
MIL-53(Fe) (with uricase)	Sensitive and rapid	Unstable and unrepeatable	[3]
Ag nanoprisms (with uricase)	Sensitive and rapid	Unstable and unrepeatable	[4]
$ZnFe_2O_4$ MNPs (with uricase)	Sensitive and rapid	Unstable and unrepeatable	[5]
Th-MOF (with uricase)	Sensitive and rapid	Unstable and unrepeatable	[6]
Ni@MnO_2 (without uricase)	Sensitive, rapid, stable and repeatable	Scarce	[7]
CoP/NF (without uricase)	Sensitive, rapid, stable and repeatable	Scarce	[8]

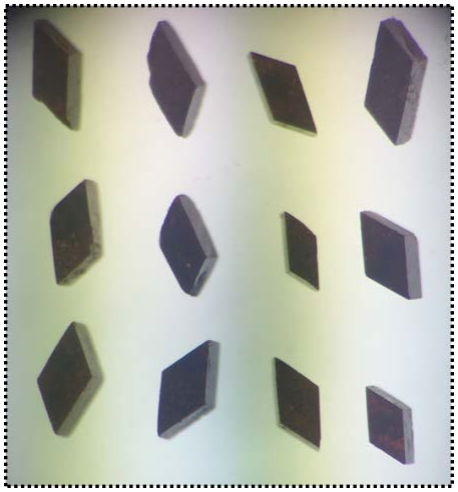


Figure S1. Crystal photograph of Ag_5PMo_{12} under optical microscope.

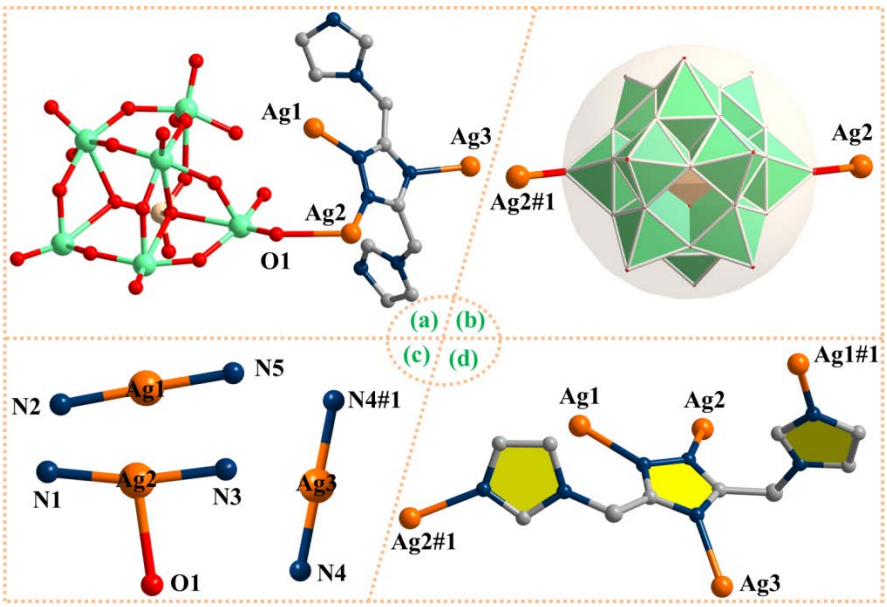


Figure S2. (a) Combined ball and stick representation of the asymmetric unit of Ag_5PMo_{12}. All the hydrogen atoms and water molecules have been omitted for clarity; (b and c) The coordination view of the PMo_{12} polyanions and the Ag ions; (d) Representation of the coordination modes of the bimt ligand.

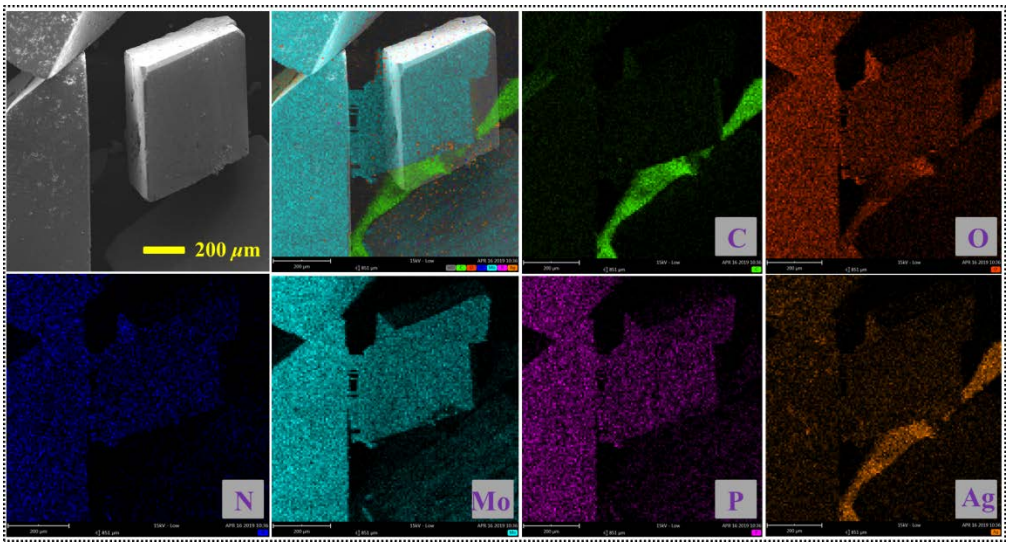
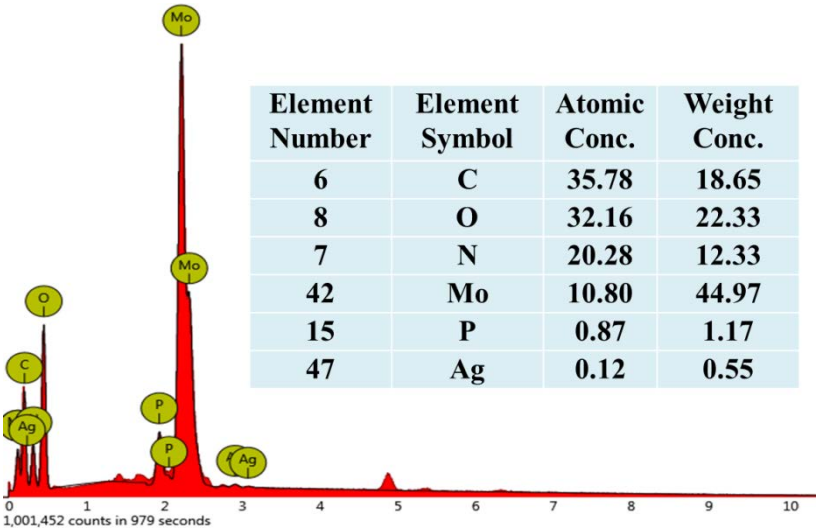
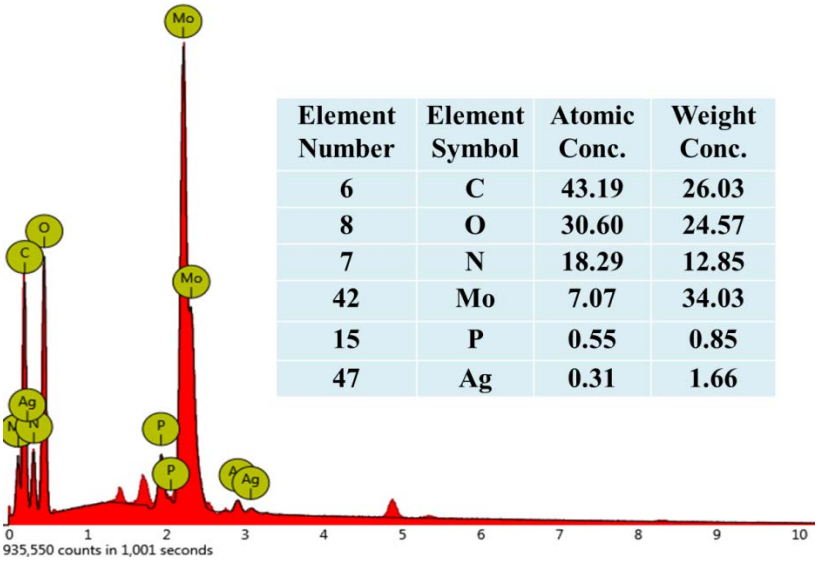


Figure S3. The corresponding EDX elemental mapping images of C, O, N, Mo, P, and Ag in Ag_5PMo_{12}.



Element Number	Element Symbol	Atomic Conc.	Weight Conc.
6	C	35.78	18.65
8	O	32.16	22.33
7	N	20.28	12.33
42	Mo	10.80	44.97
15	P	0.87	1.17
47	Ag	0.12	0.55

Figure S4. EDX spectrometry of Ag_5PMo_{12}.



Element Number	Element Symbol	Atomic Conc.	Weight Conc.
6	C	43.19	26.03
8	O	30.60	24.57
7	N	18.29	12.85
42	Mo	7.07	34.03
15	P	0.55	0.85
47	Ag	0.31	1.66

Figure S5. EDX spectrometry of Ag_5PMo_{12}@PPy.

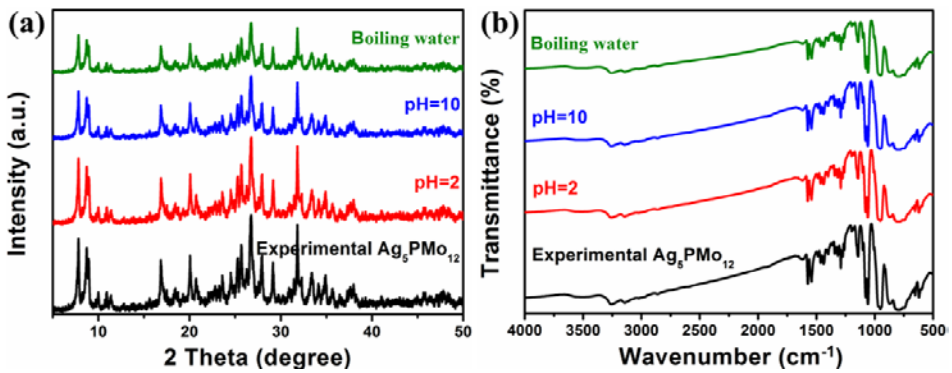


Figure S6. (a) PXRD patterns and (b) IR spectra of Ag_5PMo_{12} before and after soaked in aqueous solutions with different pH values at room temperature or immersed in boiling water for 24 h.

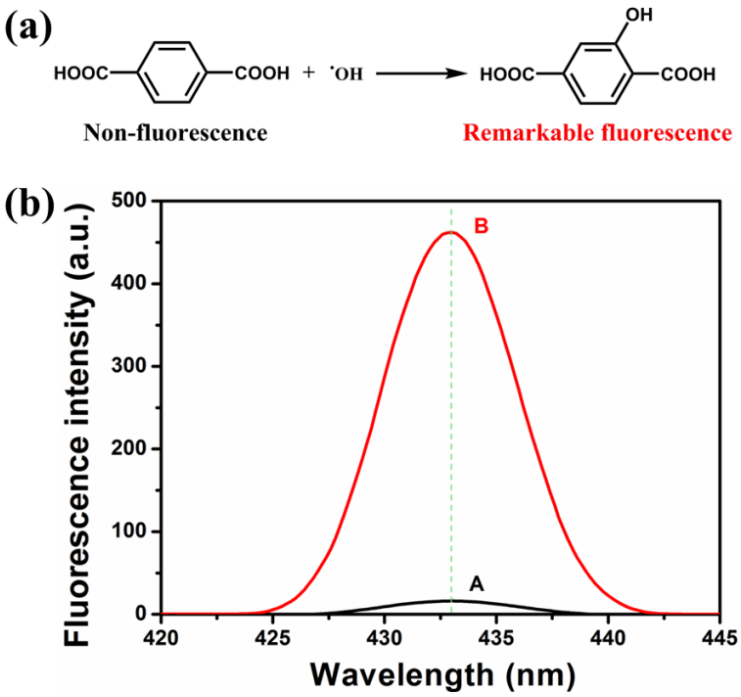


Figure S7. (a) The reaction equation of ·OH induced conversion of non-fluorescent terephthalic acid to remarkable fluorescent 2-hydroxyterephthalic acid. (b) Fluorescence spectra of TA solution (2×10^{-3} M) in the absence (A) and presence (B) of 200 μL of Ag_5PMo_{12}@PPy dispersion solution (0.6 mg.mL^{-1}) with 100 μL of H_2O_2 (10 mM).

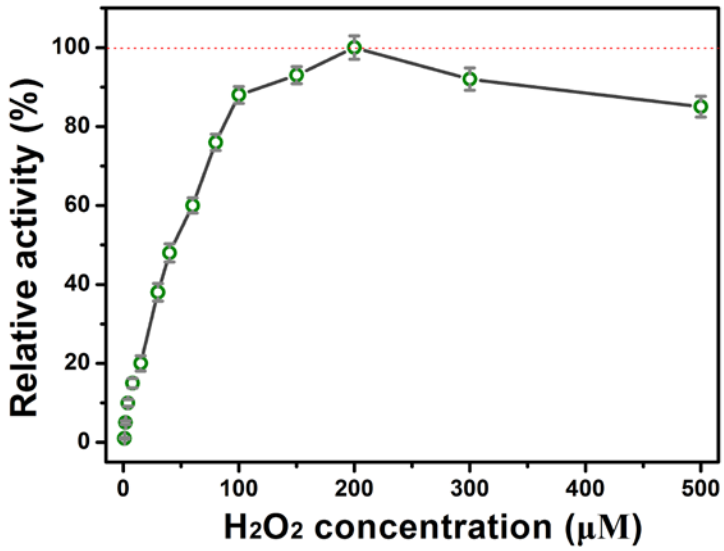


Figure S8. Dependence of the peroxidase-like activity of Ag_5PMo_{12}@PPy on H_2O_2 concentration.

Steady-state kinetics experiment

To get insight into the kinetic parameters of Ag_5PMo_{12}@PPy catalyzed reactions, the typical Michaelis–Menten model was used to evaluate the catalytic activity, and the apparent steady-state kinetic parameters were determined at the optimal condition by varying the TMB concentrations and fixing the concentration of H_2O_2 (200 μM), or varying the H_2O_2 concentrations and fixing the concentration of TMB (100 μM).

Michaelis-Menten curves were plotted according to Lineweaver-Burk plotting method by the following equation:

$$v = V_{max} \times [S]/(K_m + [S])$$

where v is the initial velocity, V_{max} represents the maximal reaction velocity, [S] corresponds to the concentration of substrate and K_m is the Michaelis constant.

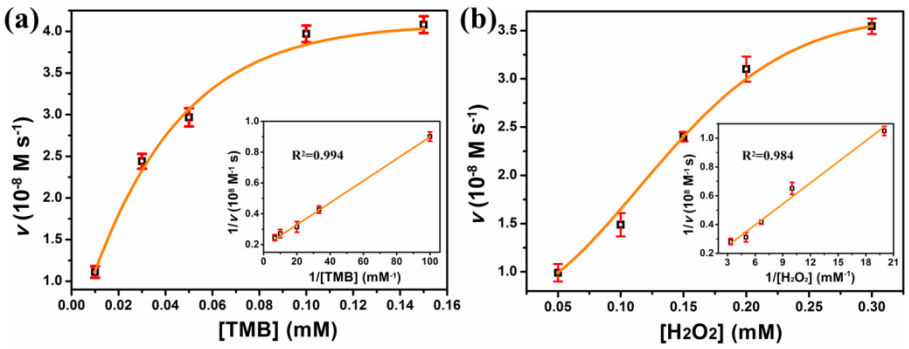


Figure S9. Steady-state kinetic assays of Ag_5PMo_{12}@PPy: (a) 200 μM H_2O_2 with varying TMB concentrations, (b) 100 μM TMB with varying H_2O_2 concentrations.

Table S2. K_m and V_{max} of Ag_5PMo_{12}@PPy and some reported peroxidase mimics.

Substrate	Enzyme mimics	K_m (mM)	V_{max} (10^{-8} M s^{-1})
H_2O_2	HRP[9]	3.7	8.71
	PW_{12}[10]	15.89	4.24×10^{-4}
	MOF-808[11]	1.06	1.39
	$Na_4H_2[Cu_4(im)_{14}][Cu_3(H_2O)_3(BiW_9O_{33})_2]$[12]	0.23	7.33
	PPy[13]	0.027	1.17
	$AgFKZSiW_{12}$[14]	1.233	5.44
	$AgFKZSiW_{12}$@PPy[14]	0.221	10.17
	Ag_5PMo_{12}@PPy	0.246	9.71

	HRP[9]	0.434	10.00
	PW_{12}[10]	0.11	43.1
	MOF-808[11]	0.0796	3.12
TMB	$Na_4H_2[Cu_4(im)_{14}][Cu_3(H_2O)_3(BiW_9O_{33})_2]$[12]	0.03	5.25
	PPy[13]	0.2157	1.29
	$AgFKZSiW_{12}$[14]	0.051	4.17
	$AgFKZSiW_{12}$@PPy[14]	0.026	5.43
	Ag_5PMo_{12}@PPy	0.034	6.83

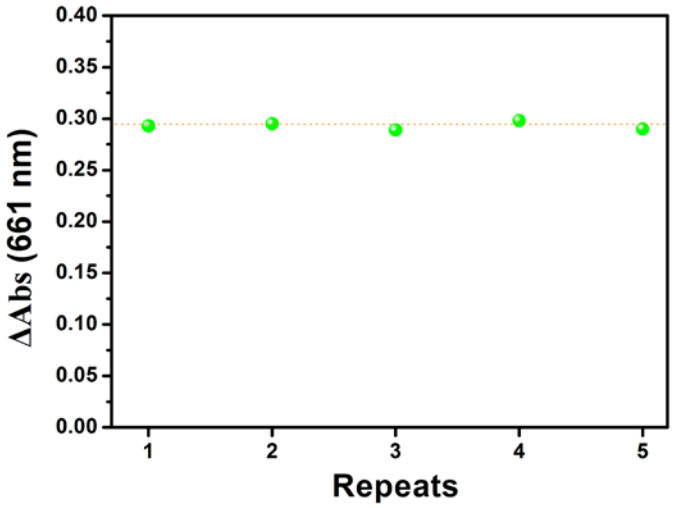


Figure S10. The repeatability evaluation of the sensing system using 50 μM UA standard solution with five repeated measurements.

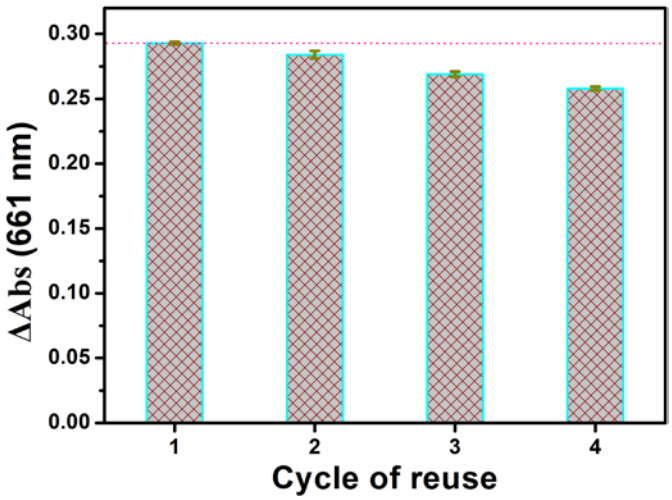


Figure S11. The ΔA661 nm signal of the sensing system, in which the same Ag_5PMo_{12}@PPy was reused repeatedly for four times.

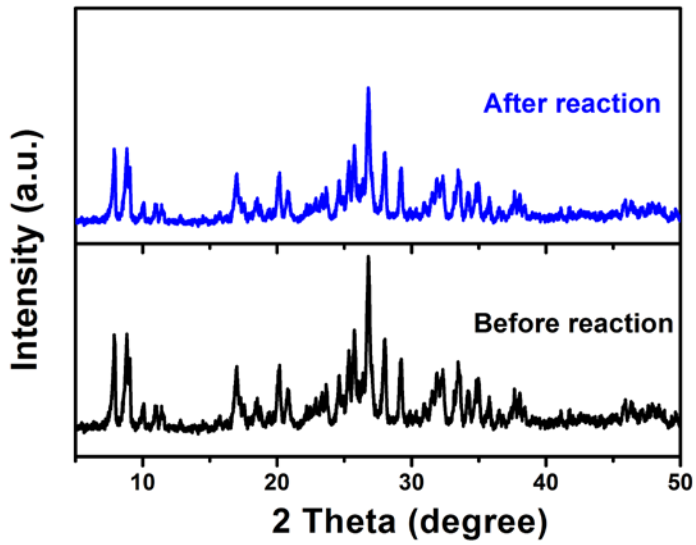


Figure S12. PXRD patterns of Ag_5PMo_{12}@PPy before and after the sensing reaction.

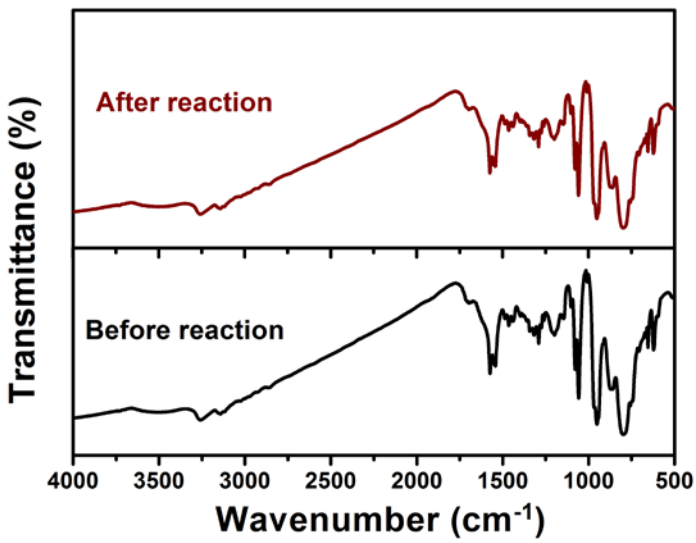


Figure S13. IR spectra of Ag_5PMo_{12}@PPy before and after the sensing reaction.

Table S3. Crystallographic data and structural refinements for Ag_5PMo_{12}.

Compound	Ag_5PMo_{12}
Chemical formula	$Ag_5C_{20}N_{14}H_{24}O_{42}PMo_{12}$
CCDC no.	1906980
Formula weight	2854.07
Temperature (K)	296(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	*P 21/n*
a(Å)	13.2277(6)
b(Å)	14.5187(7)
c(Å)	14.6344(7)

α(°)	90
β(°)	97.440(1)
γ(°)	90
V(Å^3)/Z	2786.9(2)/2
Density (g·cm^{-3})	3.477
Abs coeff. (mm^{-1})	4.465
F(000)	2728.0
Data collect θ range	1.984 to 24.998°
Reflns collected	13578
Independent reflns /R_{int}	4891/0.0186
Data/restraints/parameters	4891/114/440
Goodness-of-fit on F^2	1.046
Final R indices [I > 2δ(I)] R indices (all data)	R_1 = 0.0564, wR_2 = 0.1552 R_1 = 0.0622, wR_2 = 0.1608
Largest diff. peak and hole(e.Å-3)	3.519 and -2.437

$R_1 = \Sigma(||F_0|-|F_c||)/\Sigma|F_0|$, $wR_2 = \Sigma w(|F_0|^2-|F_c|^2)^2/\Sigma w(|F_0|^2)^2]^{1/2}$

Table S4. The BVS calculation results of Mo and Ag atoms in Ag_5PMo_{12}.

BL[a] for Mo1	**1.645 (O3)**	**1.937 (O2)**	**1.953 (O17)**	**1.830 (O14)**	**1.854 (O10)**	**2.494 (O11)**	
BL for Mo2	**1.645 (O1)**	**1.948 (O12)**	**1.836 (O2)**	**1.930 (O20)**	**1.834 (O19)**	**2.485 (O13)**	
BL for Mo3	**1.664 (O16)**	**1.840 (O17)**	**1.954 (O8)**	**1.837 (O5)**	**1.951 (O4)**	**2.401 (O21)**	
BL for Mo4	**1.850 (O4)**	**1.845 (O12)**	**2.366 (O13)**	**1.666 (O15)**	**1.930 (O16)**	**1.960 (O14)**	
BL for Mo5	**1.662 (O18)**	**1.948 (O5)**	**1.850 (O6)**	**1.945 (O19)**	**1.845 (O9)**	**2.553 (O22)**	
BL for Mo6	**1.647 (O11)**	**1.954 (O9)**	**1.948 (O10)**	**1.839 (O20)**	**1.827 (O8)**	**2.513 (O21)**	
BL for Ag1	**2.130 (N2)**	**2.101 (N5)**					
BL for Ag2	**2.504 (O1)**	**2.140 (N1)**	**2.135 (N3)**				
BL for Ag3	**2.144 (N4)**	**2.144 (N4#1)**					
BV[b] for Mo1	**1.9921**	**0.9048**	**0.8665**	**1.2083**	**1.1324**	**0.2008**	**6.3049 (total)**
BV for Mo2	**1.9921**	**0.8783**	**1.1889**	**0.9221**	**1.1953**	**0.2057**	**6.3825 (total)**
BV for Mo3	**1.8924**	**1.1760**	**0.8642**	**1.1856**	**0.8712**	**0.2582**	**6.2477 (total)**
BV for Mo4	**1.4447**	**1.1603**	**0.2838**	**1.8822**	**0.9221**	**0.8503**	**6.2434 (total)**
BV for Mo5	**1.8975**	**0.8783**	**1.1447**	**0.8855**	**1.1603**	**0.1712**	**6.1376 (total)**
BV for Mo6	**1.9814**	**0.8642**	**0.8783**	**1.1792**	**1.2181**	**0.1907**	**6.3120 (total)**

BV for Ag1	**0.4692**	**0.5074**					**0.9766 (total)**
BV for Ag2	**0.1671**	**0.4567**	**0.4629**				**1.0867 (total)**
BV for Ag3	**0.4518**	**0.4518**					**0.9036 (total)**

[a]BL= bond length, [b]BV= bond valence

Table S5. Selected bond lengths (Å) and bond angles (°) of Ag_5PMo_{12}.

Bond	Lengths	Bond	Lengths
C(1)-C(6)	1.361(17)	O(1)-Mo(2)	1.645(8)
C(1)-N(6)	1.365(16)	O(1)-Ag(2)	2.504(9)
C(1)-H(1)	0.9300	O(2)-Mo(2)	1.836(11)
C(2)-N(2)	1.313(14)	O(2)-Mo(1)#3	1.937(10)
C(2)-N(4)	1.343(14)	O(1W)-H(1A)	0.8500
C(2)-C(4)	1.508(15)	O(1W)-H(1B)	0.8500
C(3)-N(5)	1.32(2)	O(3)-Mo(1)	1.645(8)
C(3)-N(7)	1.400(17)	O(4)-Mo(4)	1.850(9)
C(3)-H(3)	0.9300	O(4)-Mo(3)	1.951(9)
C(4)-N(6)	1.469(15)	O(5)-Mo(3)	1.837(9)
C(4)-H(4A)	0.9700	O(5)-Mo(5)	1.948(9)
C(4)-H(4B)	0.9700	O(6)-Mo(5)	1.850(9)
C(5)-N(3)	1.326(16)	O(6)-Mo(4)	1.930(9)
C(5)-N(6)	1.335(16)	O(7)-P(1)	1.598(12)
C(5)-H(5)	0.9300	O(7)-O(22)#3	1.733(16)
C(6)-N(3)	1.348(15)	O(7)-Mo(5)	2.366(12)
C(6)-H(6)	0.9300	O(7)-Mo(6)	2.436(12)
C(7)-N(7)	1.478(15)	O(7)-Mo(2)	2.465(12)
C(7)-C(10)	1.502(14)	O(8)-Mo(6)#3	1.827(12)
C(7)-H(7A)	0.9700	O(8)-Mo(3)	1.954(10)
C(7)-H(7B)	0.9700	O(9)-Mo(5)	1.845(10)
C(8)-C(9)	1.33(2)	O(9)-Mo(6)	1.954(11)
C(8)-N(7)	1.332(15)	O(10)-Mo(1)	1.854(9)
C(8)-H(8)	0.9300	O(10)-Mo(6)	1.948(9)
C(9)-N(5)	1.419(19)	O(11)-Mo(6)	1.647(8)
C(9)-H(9)	0.9300	O(12)-Mo(4)	1.845(11)
C(10)-N(1)	1.321(14)	O(12)-Mo(2)#3	1.948(13)
C(10)-N(4)	1.349(14)	O(13)-P(1)	1.584(12)
N(1)-N(2)	1.358(12)	O(13)-O(22)#3	1.692(17)
N(1)-Ag(2)	2.140(8)	O(13)-O(21)#3	1.820(17)
N(2)-Ag(1)	2.130(9)	O(13)-Mo(4)	2.366(12)
N(3)-Ag(2)#1	2.135(10)	O(13)-Mo(1)	2.434(12)

N(4)-Ag(3)	2.144(9)	O(13)-Mo(2)#3	2.485(12)
N(5)-Ag(1)#2	2.101(12)	O(14)-Mo(1)	1.830(12)
O(16)-Mo(3)	1.664(9)	O(14)-Mo(4)	1.960(10)
O(17)-Mo(3)	1.840(9)	O(15)-Mo(4)	1.666(10)
O(17)-Mo(1)#3	1.953(11)	O(21)-P(1)	1.535(12)
O(18)-Mo(5)	1.662(9)	O(21)-O(22)#3	1.614(17)
O(19)-Mo(2)	1.834(12)	O(21)-O(13)#3	1.820(17)
O(19)-Mo(5)	1.945(11)	O(22)-P(1)	1.438(12)
O(20)-Mo(6)	1.839(10)	O(22)-O(21)#3	1.614(17)
O(20)-Mo(2)	1.929(10)	O(22)-O(13)#3	1.692(17)
O(21)-Mo(3)	2.400(12)	O(22)-O(7)#3	1.733(16)
O(21)-Mo(1)#3	2.494(12)	O(22)-Mo(3)#3	2.498(12)
O(21)-Mo(6)#3	2.513(12)	Mo(1)-O(17)#3	1.953(11)
O(22)-Mo(4)#3	2.499(12)	Mo(1)-O(21)#3	2.494(12)
P(1)-O(22)#3	1.438(12)	Mo(2)-O(12)#3	1.948(13)
P(1)-O(21)#3	1.535(12)	Mo(2)-O(13)#3	2.485(12)
P(1)-O(13)#3	1.584(12)	Mo(3)-O(22)#3	2.498(12)
P(1)-O(7)#3	1.598(12)	Mo(4)-O(22)#3	2.499(12)
Mo(1)-O(2)#3	1.937(10)	Mo(6)-O(8)#3	1.827(12)
Ag(1)-N(5)#4	2.101(12)	Mo(6)-O(21)#3	2.513(12)
Ag(2)-N(3)#5	2.135(10)	Ag(3)-N(4)#6	2.144(9)

Bond	**Angles**	**Bond**	**Angles**
C(6)-C(1)-N(6)	106.1(10)	N(4)-C(10)-C(7)	123.6(10)
C(6)-C(1)-H(1)	127.0	C(10)-N(1)-N(2)	106.3(8)
N(6)-C(1)-H(1)	127.0	C(10)-N(1)-Ag(2)	123.8(7)
N(2)-C(2)-N(4)	113.1(9)	N(2)-N(1)-Ag(2)	127.4(7)
N(2)-C(2)-C(4)	128.4(10)	C(2)-N(2)-N(1)	106.1(8)
N(4)-C(2)-C(4)	118.4(10)	C(2)-N(2)-Ag(1)	132.0(7)
N(5)-C(3)-N(7)	111.0(13)	N(1)-N(2)-Ag(1)	121.8(7)
N(5)-C(3)-H(3)	124.5	C(5)-N(3)-C(6)	107.1(10)
N(7)-C(3)-H(3)	124.5	C(5)-N(3)-Ag(2)#1	122.1(8)
N(6)-C(4)-C(2)	114.8(10)	C(6)-N(3)-Ag(2)#1	130.5(8)
N(6)-C(4)-H(4A)	108.6	C(2)-N(4)-C(10)	102.2(9)
C(2)-C(4)-H(4A)	108.6	C(2)-N(4)-Ag(3)	129.1(7)
N(6)-C(4)-H(4B)	108.6	C(10)-N(4)-Ag(3)	121.9(7)
C(2)-C(4)-H(4B)	108.6	C(3)-N(5)-C(9)	103.8(12)
H(4A)-C(4)-H(4B)	107.5	C(3)-N(5)-Ag(1)#2	124.3(10)
N(3)-C(5)-N(6)	109.9(11)	C(9)-N(5)-Ag(1)#2	131.9(10)

N(3)-C(5)-H(5)	125.0	C(5)-N(6)-C(1)	107.9(10)
N(6)-C(5)-H(5)	125.0	C(5)-N(6)-C(4)	123.4(11)
N(3)-C(6)-C(1)	109.0(10)	C(1)-N(6)-C(4)	128.3(11)
N(3)-C(6)-H(6)	125.5	C(8)-N(7)-C(3)	106.0(11)
C(1)-C(6)-H(6)	125.5	C(8)-N(7)-C(7)	126.4(10)
N(7)-C(7)-C(10)	108.3(9)	C(3)-N(7)-C(7)	127.1(10)
N(7)-C(7)-H(7A)	110.0	Mo(2)-O(1)-Ag(2)	139.2(5)
C(10)-C(7)-H(7A)	110.0	Mo(2)-O(2)-Mo(1)#3	138.9(7)
N(7)-C(7)-H(7B)	110.0	H(1A)-O(1W)-H(1B)	107.7
C(10)-C(7)-H(7B)	110.0	Mo(4)-O(4)-Mo(3)	138.7(5)
H(7A)-C(7)-H(7B)	108.4	Mo(3)-O(5)-Mo(5)	139.8(6)
C(9)-C(8)-N(7)	108.8(11)	Mo(5)-O(6)-Mo(4)	138.4(5)
C(9)-C(8)-H(8)	125.6	P(1)-O(7)-O(22)#3	51.0(5)
N(7)-C(8)-H(8)	125.6	P(1)-O(7)-Mo(5)	126.2(6)
C(8)-C(9)-N(5)	109.6(12)	O(22)#3-O(7)-Mo(5)	75.3(6)
C(8)-C(9)-H(9)	125.2	P(1)-O(7)-Mo(6)	121.4(6)
N(5)-C(9)-H(9)	125.2	O(22)#3-O(7)-Mo(6)	138.2(7)
N(1)-C(10)-N(4)	112.3(9)	Mo(5)-O(7)-Mo(6)	95.6(4)
N(1)-C(10)-C(7)	123.9(10)	P(1)-O(7)-Mo(2)	118.9(6)
Mo(5)-O(7)-Mo(2)	94.3(4)	O(22)#3-O(7)-Mo(2)	128.5(7)
Mo(6)-O(7)-Mo(2)	92.3(4)	O(22)#3-O(21)-Mo(6)#3	128.8(7)
Mo(6)#3-O(8)-Mo(3)	140.2(7)	O(13)#3-O(21)-Mo(6)#3	126.3(7)
Mo(5)-O(9)-Mo(6)	138.9(7)	Mo(3)-O(21)-Mo(6)#3	92.7(4)
Mo(1)-O(10)-Mo(6)	139.4(6)	Mo(1)#3-O(21)-Mo(6)#3	90.9(4)
Mo(4)-O(12)-Mo(2)#3	138.6(9)	P(1)-O(22)-O(21)#3	60.1(6)
P(1)-O(13)-O(22)#3	52.0(6)	P(1)-O(22)-O(13)#3	60.2(6)
P(1)-O(13)-O(21)#3	53.1(5)	O(21)#3-O(22)-O(13)#3	100.0(9)
O(22)#3-O(13)-O(21)#3	90.7(8)	P(1)-O(22)-O(7)#3	59.7(6)
P(1)-O(13)-Mo(4)	125.8(7)	O(21)#3-O(22)-O(7)#3	97.0(8)
O(22)#3-O(13)-Mo(4)	73.9(6)	O(13)#3-O(22)-O(7)#3	94.2(8)
O(21)#3-O(13)-Mo(4)	140.5(7)	P(1)-O(22)-Mo(3)#3	127.5(7)
P(1)-O(13)-Mo(1)	123.1(6)	O(21)#3-O(22)-Mo(3)#3	67.5(6)
O(22)#3-O(13)-Mo(1)	135.0(8)	O(13)#3-O(22)-Mo(3)#3	136.3(7)
O(21)#3-O(13)-Mo(1)	70.1(5)	O(7)#3-O(22)-Mo(3)#3	128.0(7)
Mo(4)-O(13)-Mo(1)	95.2(4)	P(1)-O(22)-Mo(4)#3	125.6(7)
P(1)-O(13)-Mo(2)#3	118.5(6)	O(21)#3-O(22)-Mo(4)#3	131.1(8)
O(22)#3-O(13)-Mo(2)#3	131.6(7)	O(13)#3-O(22)-Mo(4)#3	65.5(6)
O(21)#3-O(13)-Mo(2)#3	122.1(7)	O(7)#3-O(22)-Mo(4)#3	129.0(7)

Mo(4)-O(13)-Mo(2)#3	94.0(4)	Mo(3)#3-O(22)-Mo(4)#3	90.8(4)
Mo(1)-O(13)-Mo(2)#3	91.9(4)	O(22)-P(1)-O(22)#3	180.0
Mo(1)-O(14)-Mo(4)	138.6(9)	O(22)-P(1)-O(21)	114.3(6)
Mo(3)-O(17)-Mo(1)#3	139.6(7)	O(22)#3-P(1)-O(21)	65.7(6)
Mo(2)-O(19)-Mo(5)	139.3(7)	O(22)-P(1)-O(21)#3	65.7(6)
Mo(6)-O(20)-Mo(2)	139.5(6)	O(22)#3-P(1)-O(21)#3	114.3(6)
P(1)-O(21)-O(22)#3	54.3(6)	O(21)-P(1)-O(21)#3	180.0
P(1)-O(21)-O(13)#3	55.6(5)	O(22)-P(1)-O(13)	112.1(6)
O(22)#3-O(21)-O(13)#3	93.7(8)	O(22)#3-P(1)-O(13)	67.9(6)
P(1)-O(21)-Mo(3)	128.3(7)	O(21)-P(1)-O(13)	108.6(6)
O(22)#3-O(21)-Mo(3)	74.1(6)	O(21)#3-P(1)-O(13)	71.4(6)
O(13)#3-O(21)-Mo(3)	134.3(7)	O(22)-P(1)-O(13)#3	67.9(6)
P(1)-O(21)-Mo(1)#3	122.1(6)	O(22)#3-P(1)-O(13)#3	112.1(6)
O(22)#3-O(21)-Mo(1)#3	138.1(8)	O(21)-P(1)-O(13)#3	71.4(6)
O(13)#3-O(21)-Mo(1)#3	66.6(5)	O(21)#3-P(1)-O(13)#3	108.6(6)
Mo(3)-O(21)-Mo(1)#3	93.3(4)	O(13)-P(1)-O(13)#3	180.0(7)
P(1)-O(21)-Mo(6)#3	120.1(6)	O(22)-P(1)-O(7)#3	69.4(6)
O(21)-P(1)-O(7)#3	73.6(6)	O(22)#3-P(1)-O(7)#3	110.6(6)
O(21)#3-P(1)-O(7)#3	106.4(6)	O(19)-Mo(2)-O(20)	88.5(5)
O(13)-P(1)-O(7)#3	75.9(6)	O(2)-Mo(2)-O(20)	156.6(6)
O(13)#3-P(1)-O(7)#3	104.1(6)	O(1)-Mo(2)-O(12)#3	100.5(6)
O(22)-P(1)-O(7)	110.6(6)	O(19)-Mo(2)-O(12)#3	157.1(6)
O(22)#3-P(1)-O(7)	69.4(6)	O(2)-Mo(2)-O(12)#3	87.3(5)
O(21)-P(1)-O(7)	106.4(6)	O(20)-Mo(2)-O(12)#3	84.1(5)
O(21)#3-P(1)-O(7)	73.6(6)	O(1)-Mo(2)-O(7)	155.5(5)
O(13)-P(1)-O(7)	104.1(6)	O(19)-Mo(2)-O(7)	62.4(5)
O(13)#3-P(1)-O(7)	75.9(6)	O(2)-Mo(2)-O(7)	96.2(6)
O(7)#3-P(1)-O(7)	180.0	O(20)-Mo(2)-O(7)	63.1(4)
O(3)-Mo(1)-O(14)	102.0(6)	O(12)#3-Mo(2)-O(7)	95.1(6)
O(3)-Mo(1)-O(10)	102.5(5)	O(1)-Mo(2)-O(13)#3	157.4(5)
O(14)-Mo(1)-O(10)	92.3(5)	O(19)-Mo(2)-O(13)#3	97.1(5)
O(3)-Mo(1)-O(2)#3	101.9(6)	O(2)-Mo(2)-O(13)#3	64.4(5)
O(14)-Mo(1)-O(2)#3	88.3(5)	O(20)-Mo(2)-O(13)#3	92.4(5)
O(10)-Mo(1)-O(2)#3	154.9(6)	O(12)#3-Mo(2)-O(13)#3	61.8(5)
O(3)-Mo(1)-O(17)#3	101.1(5)	O(7)-Mo(2)-O(13)#3	46.6(4)
O(14)-Mo(1)-O(17)#3	156.5(6)	O(16)-Mo(3)-O(5)	102.3(6)
O(10)-Mo(1)-O(17)#3	87.5(4)	O(16)-Mo(3)-O(17)	103.8(6)
O(2)#3-Mo(1)-O(17)#3	82.3(5)	O(5)-Mo(3)-O(17)	92.8(4)

O(3)-Mo(1)-O(13)	158.5(5)	O(16)-Mo(3)-O(4)	100.1(6)
O(14)-Mo(1)-O(13)	62.9(6)	O(5)-Mo(3)-O(4)	87.2(4)
O(10)-Mo(1)-O(13)	93.7(5)	O(17)-Mo(3)-O(4)	155.5(5)
O(2)#3-Mo(1)-O(13)	64.4(5)	O(16)-Mo(3)-O(8)	102.1(6)
O(17)#3-Mo(1)-O(13)	93.6(5)	O(5)-Mo(3)-O(8)	154.7(6)
O(3)-Mo(1)-O(21)#3	157.9(4)	O(17)-Mo(3)-O(8)	87.8(4)
O(14)-Mo(1)-O(21)#3	97.0(6)	O(4)-Mo(3)-O(8)	82.1(4)
O(10)-Mo(1)-O(21)#3	65.4(4)	O(16)-Mo(3)-O(21)	161.0(6)
O(2)#3-Mo(1)-O(21)#3	89.6(6)	O(5)-Mo(3)-O(21)	93.8(5)
O(17)#3-Mo(1)-O(21)#3	61.6(5)	O(17)-Mo(3)-O(21)	64.9(5)
O(13)-Mo(1)-O(21)#3	43.3(4)	O(4)-Mo(3)-O(21)	90.7(4)
O(1)-Mo(2)-O(19)	102.1(6)	O(8)-Mo(3)-O(21)	63.7(5)
O(1)-Mo(2)-O(2)	103.3(6)	O(16)-Mo(3)-O(22)#3	160.0(6)
O(19)-Mo(2)-O(2)	91.1(6)	O(5)-Mo(3)-O(22)#3	66.3(4)
O(1)-Mo(2)-O(20)	99.7(5)	O(17)-Mo(3)-O(22)#3	93.5(5)
O(8)-Mo(3)-O(22)#3	88.4(5)	O(4)-Mo(3)-O(22)#3	64.2(4)
O(21)-Mo(3)-O(22)#3	38.4(4)	O(19)-Mo(5)-O(7)	63.3(5)
O(15)-Mo(4)-O(12)	101.6(8)	O(5)-Mo(5)-O(7)	92.4(4)
O(15)-Mo(4)-O(4)	101.6(5)	O(11)-Mo(6)-O(8)#3	102.7(5)
O(12)-Mo(4)-O(4)	93.2(5)	O(11)-Mo(6)-O(20)	103.1(5)
O(15)-Mo(4)-O(6)	100.3(6)	O(8)#3-Mo(6)-O(20)	92.3(5)
O(12)-Mo(4)-O(6)	157.3(6)	O(11)-Mo(6)-O(10)	100.8(5)
O(4)-Mo(4)-O(6)	88.3(4)	O(8)#3-Mo(6)-O(10)	87.9(4)
O(15)-Mo(4)-O(14)	100.7(7)	O(20)-Mo(6)-O(10)	155.5(5)
O(12)-Mo(4)-O(14)	85.9(5)	O(11)-Mo(6)-O(9)	100.7(5)
O(4)-Mo(4)-O(14)	157.4(6)	O(8)#3-Mo(6)-O(9)	156.0(6)
O(6)-Mo(4)-O(14)	84.1(4)	O(20)-Mo(6)-O(9)	87.5(5)
O(15)-Mo(4)-O(13)	158.7(5)	O(10)-Mo(6)-O(9)	82.7(5)
O(12)-Mo(4)-O(13)	65.5(6)	O(11)-Mo(6)-O(7)	157.2(4)
O(4)-Mo(4)-O(13)	96.2(4)	O(8)#3-Mo(6)-O(7)	97.2(5)
O(6)-Mo(4)-O(13)	91.7(4)	O(20)-Mo(6)-O(7)	64.8(5)
O(14)-Mo(4)-O(13)	62.9(6)	O(10)-Mo(6)-O(7)	90.9(5)
O(15)-Mo(4)-O(22)#3	160.5(6)	O(9)-Mo(6)-O(7)	61.1(5)
O(12)-Mo(4)-O(22)#3	93.8(7)	O(11)-Mo(6)-O(21)#3	157.8(4)
O(4)-Mo(4)-O(22)#3	65.3(4)	O(8)#3-Mo(6)-O(21)#3	62.6(5)
O(6)-Mo(4)-O(22)#3	66.3(4)	O(20)-Mo(6)-O(21)#3	94.5(5)
O(14)-Mo(4)-O(22)#3	92.2(6)	O(10)-Mo(6)-O(21)#3	63.9(4)
O(13)-Mo(4)-O(22)#3	40.6(4)	O(9)-Mo(6)-O(21)#3	93.5(5)

O(18)-Mo(5)-O(9)	102.4(5)	O(7)-Mo(6)-O(21)#3	44.6(4)
O(18)-Mo(5)-O(6)	101.9(6)	N(5)#4-Ag(1)-N(2)	178.3(5)
O(9)-Mo(5)-O(6)	92.4(5)	N(3)#5-Ag(2)-N(1)	165.8(4)
O(18)-Mo(5)-O(19)	102.0(6)	N(3)#5-Ag(2)-O(1)	88.9(3)
O(9)-Mo(5)-O(19)	88.0(4)	N(1)-Ag(2)-O(1)	104.0(3)
O(6)-Mo(5)-O(19)	155.4(5)	N(4)#6-Ag(3)-N(4)	180.0(5)
O(18)-Mo(5)-O(5)	100.9(5)	O(19)-Mo(5)-O(5)	82.5(4)
O(9)-Mo(5)-O(5)	156.2(5)	O(18)-Mo(5)-O(7)	158.9(5)
O(6)-Mo(5)-O(5)	87.5(4)	O(9)-Mo(5)-O(7)	63.8(5)
O(6)-Mo(5)-O(7)	94.9(5)		

Symmetry transformations used to generate equivalent atoms: #1 x-1/2, -y+1/2, z-1/2; #2 -x+1/2, y-1/2, -z+3/2; #3 -x, -y, -z+2; #4 -x+1/2, y+1/2, -z+3/2; #5 x+1/2, -y+1/2, z+1/2; #6 -x+1, -y, -z+1

Section 2. References

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