Supporting Information File

Assembly of polyoxometalate-based inorganic-organic compounds from silver-Schiff base building blocks: synthesis, crystal structures and luminescent properties

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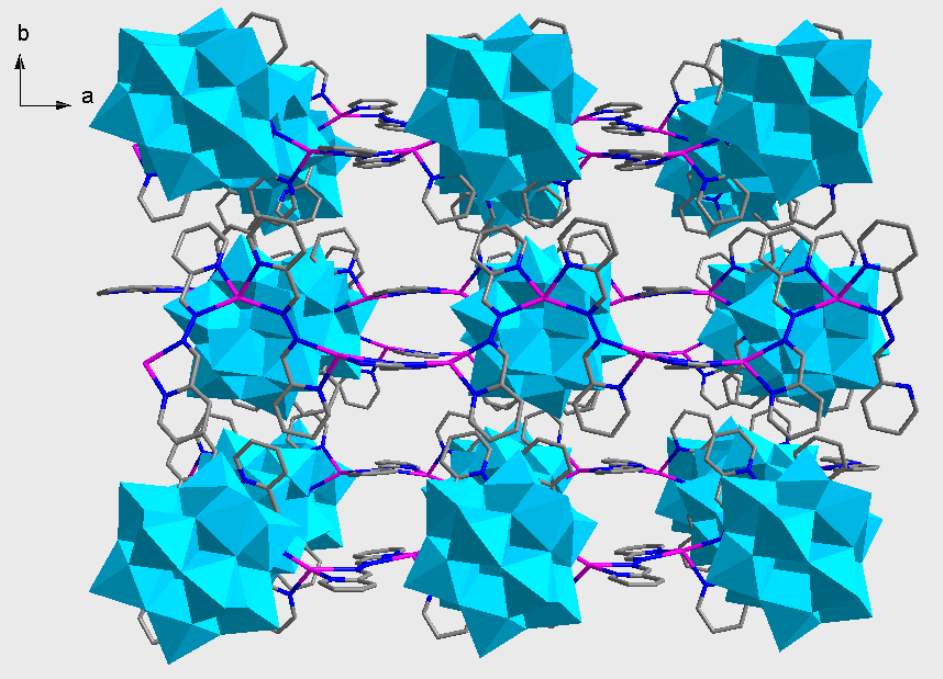

Figure S1. View of 3D supramolecular structure of **1**.

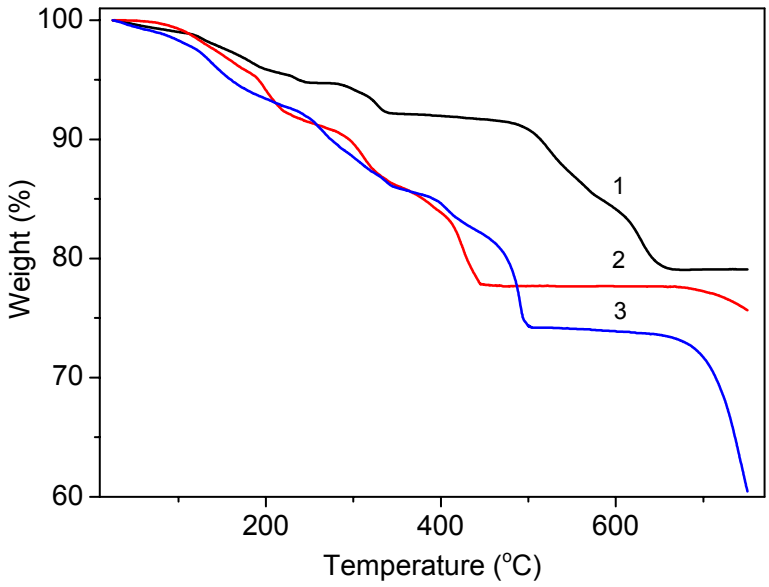

Figure S2. TGA curves for compounds **1**–**3**.

Table S1. Selected bond lengths (Å) for compound **1**

bond	length	bond	length
P(1)–O(39)	1.504(7)	P(1)–O(38)	1.525(8)
P(1)–O(40)	1.521(7)	P(1)–O(37)	1.517(8)
P(1)–O(39')	1.521(9)	P(1)–O(38')	1.520(9)
P(1)–O(40')	1.512(9)	P(1)–O(37')	1.515(9)
W(1)–O(1)	1.704(9)	W(1)–O(15)	1.873(10)
W(1)–O(16)	1.892(9)	W(1)–O(14)	1.893(11)
W(1)–O(13)	1.925(11)	W(1)–O(38)	2.419(10)
W(1)–O(40')	2.53(3)	W(2)–O(2)	1.648(10)
W(2)–O(17)	1.849(10)	W(2)–O(19)	1.907(10)
W(2)–O(13)	1.923(11)	W(2)–O(18)	1.927(12)
W(2)–O(38)	2.483(10)	W(2)–O(37')	2.57(3)
W(3)–O(3)	1.669(10)	W(3)–O(20)	1.867(10)
W(3)–O(19)	1.895(11)	W(3)–O(21)	1.910(10)
W(3)–O(14)	1.928(11)	W(3)–O(38)	2.464(10)
W(3)–O(39')	2.64(3)	W(4)–O(4)	1.674(9)
W(4)–O(25)	1.869(11)	W(4)–O(24)	1.909(11)
W(4)–O(22)	1.922(11)	W(4)–O(23)	1.936(11)
W(4)–O(37)	2.495(10)	W(4)–O(38')	2.56(3)
W(5)–O(5)	1.690(9)	W(5)–O(26)	1.875(10)
W(5)–O(23)	1.886(11)	W(5)–O(17)	1.938(10)
W(5)–O(27)	1.943(11)	W(5)–O(37)	2.458(11)
W(5)–O(37')	2.53(3)	W(6)–O(6)	1.666(11)
W(6)–O(16)	1.889(9)	W(6)–O(22)	1.899(10)
W(6)–O(27)	1.901(10)	W(6)–O(28)	1.908(10)
W(6)–O(37)	2.423(10)	W(6)–O(40')	2.50(3)
W(7)–O(7)	1.695(9)	W(7)–O(31)	1.866(11)
W(7)–O(30)	1.902(10)	W(7)–O(25)	1.911(11)
W(7)–O(29)	1.916(12)	W(7)–O(40)	2.518(10)
W(7)–O(38')	2.63(3)	W(8)–O(8)	1.689(9)
W(8)–O(33)	1.886(11)	W(8)–O(21)	1.887(11)
W(8)–O(30)	1.901(10)	W(8)–O(32)	1.913(10)
W(8)–O(40)	2.455(9)	W(8)–O(39')	2.47(3)
W(9)–O(9)	1.702(10)	W(9)–O(29)	1.873(10)
W(9)–O(28)	1.883(10)	W(9)–O(15)	1.926(10)

W(9)–O(33)	1.949(10)	W(9)–O(40)	2.415(10)
W(9)–O(40')	2.48(3)	W(10)–O(10)	1.639(10)
W(10)–O(24)	1.864(10)	W(10)–O(34)	1.884(10)
W(10)–O(31)	1.917(10)	W(10)–O(35)	1.923(9)
W(10)–O(38')	2.35(3)	W(10)–O(39)	2.485(10)
W(11)–O(11)	1.681(9)	W(11)–O(18)	1.859(11)
W(11)–O(26)	1.897(10)	W(11)–O(36)	1.900(9)
W(11)–O(34)	1.919(10)	W(11)–O(37')	2.42(3)
W(11)–O(39)	2.504(11)	W(12)–O(12)	1.673(9)
W(12)–O(32)	1.875(10)	W(12)–O(35)	1.902(9)
W(12)–O(20)	1.920(10)	W(12)–O(36)	1.930(9)
W(12)–O(39')	2.40(3)	W(12)–O(39)	2.436(10)
Ag(1)–N(1)	2.298(13)	Ag(1)–N(6)	2.309(13)
Ag(1)–N(2)	2.363(13)	Ag(1)–N(5)	2.408(15)
Ag(2)–N(10)	2.298(12)	Ag(2)–N(8)	2.326(15)
Ag(2)–N(7)	2.328(13)	Ag(2)–N(9)	2.406(14)
Ag(3)–N(4A)	2.267(12)	Ag(3)–N(11)	2.321(12)
Ag(3)–N(12)	2.333(13)	Ag(3)–N(3A)	2.348(13)

Symmetry code A: $1 + x, y, z$.

Table S2. Selected bond angles (°) for compound **1**

bond angle	degree	bond angle	degree
O(40')–P(1)–O(37')	116(2)	O(39)–P(1)–O(37)	112.2(6)
O(40')–P(1)–O(38')	115.0(19)	O(37')–P(1)–O(38')	101.2(19)
O(39)–P(1)–O(40)	111.2(6)	O(37)–P(1)–O(40)	109.2(6)
O(40')–P(1)–O(39')	113.6(19)	O(37')–P(1)–O(39')	108.6(19)
O(38')–P(1)–O(39')	100.8(18)	O(39)–P(1)–O(38)	110.4(6)
O(37)–P(1)–O(38)	107.7(6)	O(40)–P(1)–O(38)	106.0(6)
N(1)–Ag(1)–N(6)	139.1(5)	N(1)–Ag(1)–N(2)	72.8(5)
N(6)–Ag(1)–N(2)	146.6(5)	N(1)–Ag(1)–N(5)	128.0(6)
N(6)–Ag(1)–N(5)	69.6(5)	N(2)–Ag(1)–N(5)	99.9(5)
N(10)–Ag(2)–N(8)	140.7(5)	N(10)–Ag(2)–N(7)	139.4(5)
N(8)–Ag(2)–N(7)	71.9(5)	N(10)–Ag(2)–N(9)	72.3(4)
N(8)–Ag(2)–N(9)	94.4(5)	N(7)–Ag(2)–N(9)	141.6(5)
N(4)–Ag(3)–N(11A)	138.5(4)	N(4)–Ag(3)–N(12A)	133.6(5)
N(11)–Ag(3)–N(12)	72.4(5)	N(4A)–Ag(3)–N(3A)	70.7(5)
N(11)–Ag(3)–N(3A)	138.9(5)	N(12)–Ag(3)–N(3A)	109.9(5)

Symmetry code A: 1 + *x*, *y*, *z*.

Table S3. Hydrogen bond parameters (Å, º) of compound **1**

D–H···A	D(D–H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
C(4)–H(4A)···O(8)	0.93	2.48	3.38(2)	164	$-1+x, y, z$
C(15)–H(15A)···O(7)	0.93	2.56	3.34(2)	141	$1-x, 1-y, 1-z$
C(19)–H(19A)···O(42)	0.93	2.43	3.30(2)	156	$-1+x, y, z$
C(30)–H(30A)···O(43)	0.93	2.36	3.19(2)	148	
C(33)–H(33A)···O(12)	0.93	2.51	3.38(2)	156	
C(35)–H(35A)···O(35)	0.93	2.58	3.46(2)	158	$1-x, 1-y, 1-z$
C(39)–H(39B)···O(1)	0.96	2.52	3.35(4)	144	$1-x, -1/2+y, 1/2-z$
C(41)–H(41C)···O(42)	0.96	2.45	2.80(3)	102	

Table S4. Selected bond lengths (Å) for compound **2**

bond	length	bond	length
P(1)–O(39)	1.525(7)	P(1)–O(38)	1.537(6)
P(1)–O(40)	1.539(7)	P(1)–O(37)	1.541(7)
Mo(1)–O(1)	1.685(7)	Mo(1)–O(13)	1.839(6)
Mo(1)–O(14)	1.846(7)	Mo(1)–O(15)	2.007(7)
Mo(1)–O(16)	1.980(7)	Mo(1)–O(37)	2.448(6)
Mo(2)–O(2)	1.683(7)	Mo(2)–O(15)	1.828(7)
Mo(2)–O(17)	1.835(7)	Mo(2)–O(18)	2.008(7)
Mo(2)–O(19)	2.019(7)	Mo(2)–O(37)	2.420(6)
Mo(3)–O(3)	1.681(7)	Mo(3)–O(20)	1.836(7)
Mo(3)–O(18)	1.849(7)	Mo(3)–O(14)	1.990(7)
Mo(3)–O(21)	1.994(6)	Mo(3)–O(37)	2.422(7)
Mo(4)–O(4)	1.662(7)	Mo(4)–O(21)	1.831(7)
Mo(4)–O(24)	1.841(7)	Mo(4)–O(22)	1.975(7)
Mo(4)–O(23)	1.994(7)	Mo(4)–O(38)	2.440(7)
Mo(5)–O(5)	1.681(7)	Mo(5)–O(25)	1.835(7)
Mo(5)–O(26)	1.854(7)	Mo(5)–O(13)	1.990(7)
Mo(5)–O(24)	1.998(7)	Mo(5)–O(38)	2.423(6)
Mo(6)–O(6)	1.654(7)	Mo(6)–O(27)	1.823(7)
Mo(6)–O(23)	1.852(7)	Mo(6)–O(26)	1.994(7)
Mo(6)–O(28)	2.006(7)	Mo(6)–O(38)	2.430(6)
Mo(7)–O(7)	1.670(7)	Mo(7)–O(29)	1.836(7)
Mo(7)–O(30)	1.849(7)	Mo(7)–O(31)	1.991(7)
Mo(7)–O(27)	2.021(7)	Mo(7)–O(39)	2.450(7)
Mo(8)–O(8)	1.670(7)	Mo(8)–O(19)	1.815(7)
Mo(8)–O(33)	1.838(7)	Mo(8)–O(32)	1.992(7)
Mo(8)–O(29)	2.007(7)	Mo(8)–O(39)	2.454(6)
Mo(9)–O(9)	1.670(7)	Mo(9)–O(22)	1.843(7)
Mo(9)–O(31)	1.847(7)	Mo(9)–O(20)	1.995(7)
Mo(9)–O(33)	1.998(7)	Mo(9)–O(39)	2.415(6)
Mo(10)–O(10)	1.677(7)	Mo(10)–O(28)	1.821(7)
Mo(10)–O(35)	1.853(7)	Mo(10)–O(30)	1.968(7)
Mo(10)–O(34)	2.003(7)	Mo(10)–O(40)	2.437(6)
Mo(11)–O(11)	1.681(7)	Mo(11)–O(32)	1.826(7)
Mo(11)–O(34)	1.856(7)	Mo(11)–O(36)	1.986(7)

Mo(11)–O(17)	2.011(7)	Mo(11)–O(40)	2.439(6)
Mo(12)–O(12)	1.673(7)	Mo(12)–O(16)	1.842(7)
Mo(12)–O(36)	1.855(7)	Mo(12)–O(35)	1.984(7)
Mo(12)–O(25)	1.995(6)	Mo(12)–O(40)	2.426(6)
Ag(1)–N(1)	2.244(9)	Ag(1)–N(2)	2.519(9)
Ag(1)–N(3)	2.345(10)	Ag(1)–N(4)	2.354(10)
Ag(2)–N(5)	2.455(9)	Ag(2)–N(6)	2.293(10)
Ag(2)–N(7)	2.285(12)	Ag(2)–N(8)	2.242(13)
Ag(3)–N(9)	2.296(11)	Ag(3)–N(10)	2.348(10)
Ag(3)–N(11)	2.58(2)	Ag(3)–N(12)	2.192(14)

Table S5. Selected bond angles (°) for compound **2**

bond angle	degree	bond angle	degree
O(39)–P(1)–O(38)	109.7(4)	O(39)–P(1)–O(40)	109.3(4)
O(38)–P(1)–O(40)	109.8(4)	O(39)–P(1)–O(37)	108.4(4)
O(38)–P(1)–O(37)	109.9(4)	O(40)–P(1)–O(37)	109.7(4)
N(1)–Ag(1)–N(3)	117.8(4)	N(1)–Ag(1)–N(4)	158.6(3)
N(3)–Ag(1)–N(4)	70.2(4)	N(1)–Ag(1)–N(2)	70.3(3)
N(3)–Ag(1)–N(2)	155.6(3)	N(4)–Ag(1)–N(2)	111.3(3)
N(8)–Ag(2)–N(7)	107.9(4)	N(8)–Ag(2)–N(6)	127.1(4)
N(7)–Ag(2)–N(6)	112.9(4)	N(8)–Ag(2)–N(5)	106.1(4)
N(7)–Ag(2)–N(5)	130.6(3)	N(6)–Ag(2)–N(5)	70.4(3)
N(12)–Ag(3)–N(9)	158.2(4)	N(12)–Ag(3)–N(10)	122.9(4)
N(9)–Ag(3)–N(10)	72.3(4)	N(12)–Ag(3)–N(11)	88.5(7)
N(9)–Ag(3)–N(11)	92.3(6)	N(10)–Ag(3)–N(11)	129.1(5)

Table S6. Hydrogen bond parameters (Å, º) of compound **2**

D–H···A	D(D–H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
C(7)–H(7A)···O(31)	0.93	2.56	3.372(16)	146	$1 + x, y, z$
C(8)–H(8A)···O(23)	0.93	2.54	3.436(16)	161	$1 + x, y, z$
C(22)–H(22B)···O(6)	0.96	2.40	3.150(17)	134	$1 + x, -1 + y, z$
C(22)–H(22C)···O(16)	0.96	2.56	3.374(17)	143	$x, -1 + y, z$
C(25)–H(25A)···O(5)	0.93	2.54	3.37(2)	148	$-4 - x, 4 - y, -z$
C(26)–H(26A)···O(12)	0.93	2.50	3.345(16)	152	$-4 - x, 4 - y, -z$
C(30)–H(30A)···O(13)	0.96	2.45	3.31(3)	149	
C(32)–H(32A)···O(12)	0.96	2.33	3.259(16)	163	$x, -1 + y, z$
C(32)–H(32C)···O(3)	0.96	2.58	3.252(14)	127	

Table S7. Selected bond lengths (Å) for compound **3**

bond	length	bond	length
Si(1)–O(19)	1.652(16)	Si(1)–O(20)	1.522(16)
Si(1)–O(21)	1.669(17)	Si(1)–O(22)	1.699(17)
Mo(1)–O(1)	1.659(11)	Mo(1)–O(7')	1.79(2)
Mo(1)–O(9)	1.839(11)	Mo(1)–O(7)	1.90(2)
Mo(1)–O(13A)	1.965(17)	Mo(1)–O(13A')	2.097(18)
Mo(1)–O(8)	2.003(12)	Mo(1)–O(22)	2.289(17)
Mo(1)–O(20)	2.472(16)	Mo(2)–O(2)	1.678(11)
Mo(2)–O(12)	1.828(12)	Mo(2)–O(10')	1.85(2)
Mo(2)–O(10)	1.88(2)	Mo(2)–O(9)	1.978(11)
Mo(2)–O(11')	2.01(2)	Mo(2)–O(11)	2.09(2)
Mo(2)–O(19)	2.315(17)	Mo(2)–O(20)	2.424(17)
Mo(3)–O(3)	1.680(11)	Mo(3)–O(8)	1.803(12)
Mo(3)–O(15A')	1.82(2)	Mo(3)–O(15A)	1.902(18)
Mo(3)–O(12)	1.986(11)	Mo(3)–O(17A')	2.01(2)
Mo(3)–O(17)	2.06(2)	Mo(3)–O(21A)	2.301(17)
Mo(3)–O(20)	2.462(17)	Mo(4)–O(4)	1.663(10)
Mo(4)–O(13)	1.692(17)	Mo(4)–O(14')	1.77(2)
Mo(4)–O(10')	1.82(2)	Mo(4)–O(14)	1.95(2)
Mo(4)–O(18A')	1.95(2)	Mo(4)–O(13')	2.03(2)
Mo(4)–O(18A)	2.08(2)	Mo(4)–O(10)	2.20(3)
Mo(4)–O(22A)	2.383(17)	Mo(4)–O(19)	2.427(17)
Mo(5)–O(11')	1.65(2)	Mo(5)–O(5)	1.668(10)
Mo(5)–O(16')	1.77(2)	Mo(5)–O(15')	1.847(19)
Mo(5)–O(16)	1.93(2)	Mo(5)–O(14')	1.94(2)
Mo(5)–O(11)	2.01(2)	Mo(5)–O(14)	2.07(2)
Mo(5)–O(15)	2.19(2)	Mo(5)–O(21)	2.391(17)
Mo(5)–O(19)	2.402(16)	Mo(6)–O(17')	1.63(2)
Mo(6)–O(6)	1.671(10)	Mo(6)–O(18')	1.76(2)
Mo(6)–O(7')	1.87(2)	Mo(6)–O(16')	1.96(2)
Mo(6)–O(18)	2.00(2)	Mo(6)–O(17)	2.04(2)
Mo(6)–O(16)	2.10(2)	Mo(6)–O(7)	2.18(2)
Mo(6)–O(22)	2.408(17)	Mo(6)–O(21)	2.437(17)
Ag(1)–N(1)	2.420(14)	Ag(1)–N(2)	2.358(13)
Ag(1)–N(5)	2.26(2)	Ag(1)–N(6)	2.33(2)

Ag(2)–N(3)	2.482(12)	Ag(2)–N(4)	2.208(14)
Ag(2)–N(7)	2.130(16)		

Table S8. Selected bond angles (°) for compound **3**

bond angle	degree	bond angle	degree
O(20A)–Si(1)–O(19)	114.1(9)	O(20)–Si(1)–O(21)	111.7(8)
O(19A)–Si(1)–O(21)	107.5(8)	O(20A)–Si(1)–O(22)	110.9(8)
O(19)–Si(1)–O(22)	106.2(8)	O(21A)–Si(1)–O(22)	106.0(8)
N(2)–Ag(1)–N(1)	71.1(5)	N(6)–Ag(1)–N(1)	102.2(6)
N(5)–Ag(1)–N(1)	109.2(7)	N(6)–Ag(1)–N(2)	115.5(6)
N(5)–Ag(1)–N(2)	131.5(8)	N(5)–Ag(1)–N(6)	111.7(9)
N(7)–Ag(2)–N(4)	171.8(6)	N(7)–Ag(2)–N(3)	112.8(6)
N(4)–Ag(2)–N(3)	71.8(4)		

Table S9. Hydrogen bond parameters (Å, º) of compound **3**

D–H···A	D(D–H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformation for A
C(1)–H(1A)···O(11)	0.93	2.36	3.13(3)	140	$1-x, 1-y, 1-z$
C(6)–H(6A)···O(5)	0.93	2.60	3.24(2)	126	$-1+x, y, z$
C(7)–H(7A)···O(4)	0.93	2.35	3.28(2)	175	
C(9)–H(9A)···O(13')	0.93	2.33	3.25(3)	171	
C(11)–H(11A)···O(1)	0.93	2.47	3.27(2)	144	$-1+x, -1+y, z$
C(14)–H(14B)···O(11)	0.96	2.48	3.40(4)	159	
C(18)–H(18C)···O(8)	0.96	2.51	3.26(2)	134	$-1+x, y, 1+z$
C(18)–H(18C)···O(15)	0.96	2.47	3.24(3)	137	$-x, -y, 1-z$
C(18)–H(18C)···O(15')	0.96	2.49	3.38(3)	154	$-x, -y, 1-z$
C(20)–H(20A)···O(12)	0.96	2.41	3.33(3)	159	$-x, 1-y, 1-z$
C(20)–H(20C)···O(3)	0.96	2.39	3.31(3)	159	$-1+x, y, 1+z$