Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

The influence of pendant 2-[1,2,4]triazol-4-yl-ethylamine and symmetrical bis(pyrazol) ligands on dimensional extension of POM-based compounds†

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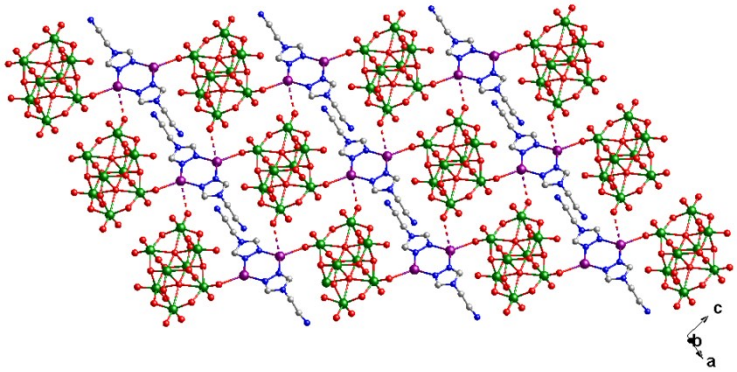

Fig. S1. The 2D supramolecular layer of compound **2** through hydrogen bonding interactions (O5···Ag1 = 2.923 Å).

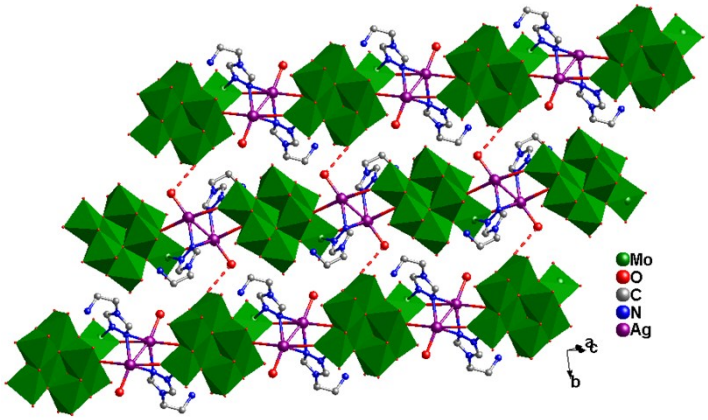

Fig. S2. The 2D supramolecular layer of compound **3** through hydrogen bonding interactions (O1W···O7 = 2.868 Å).

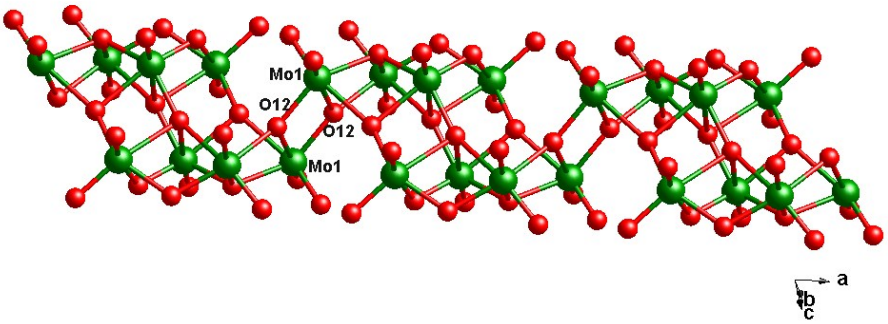

Fig. S3. The 1D inorganic Mo-chain of **4** by adjacent β-Mo_8 anions connecting each other through Mo1-O12 bonds.

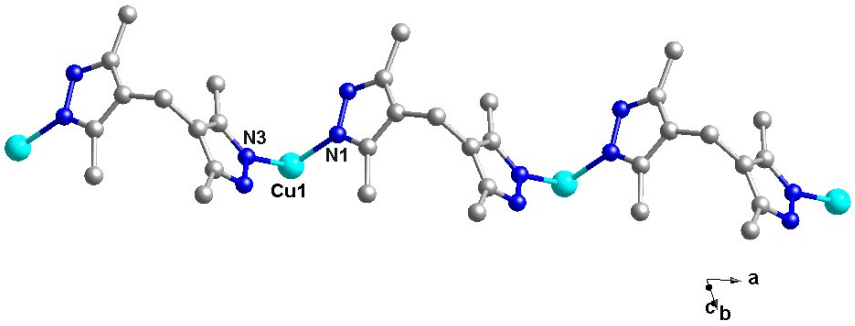

Fig. S4. The 1D zigzag Cu-H_2bdpm chain of **4**.

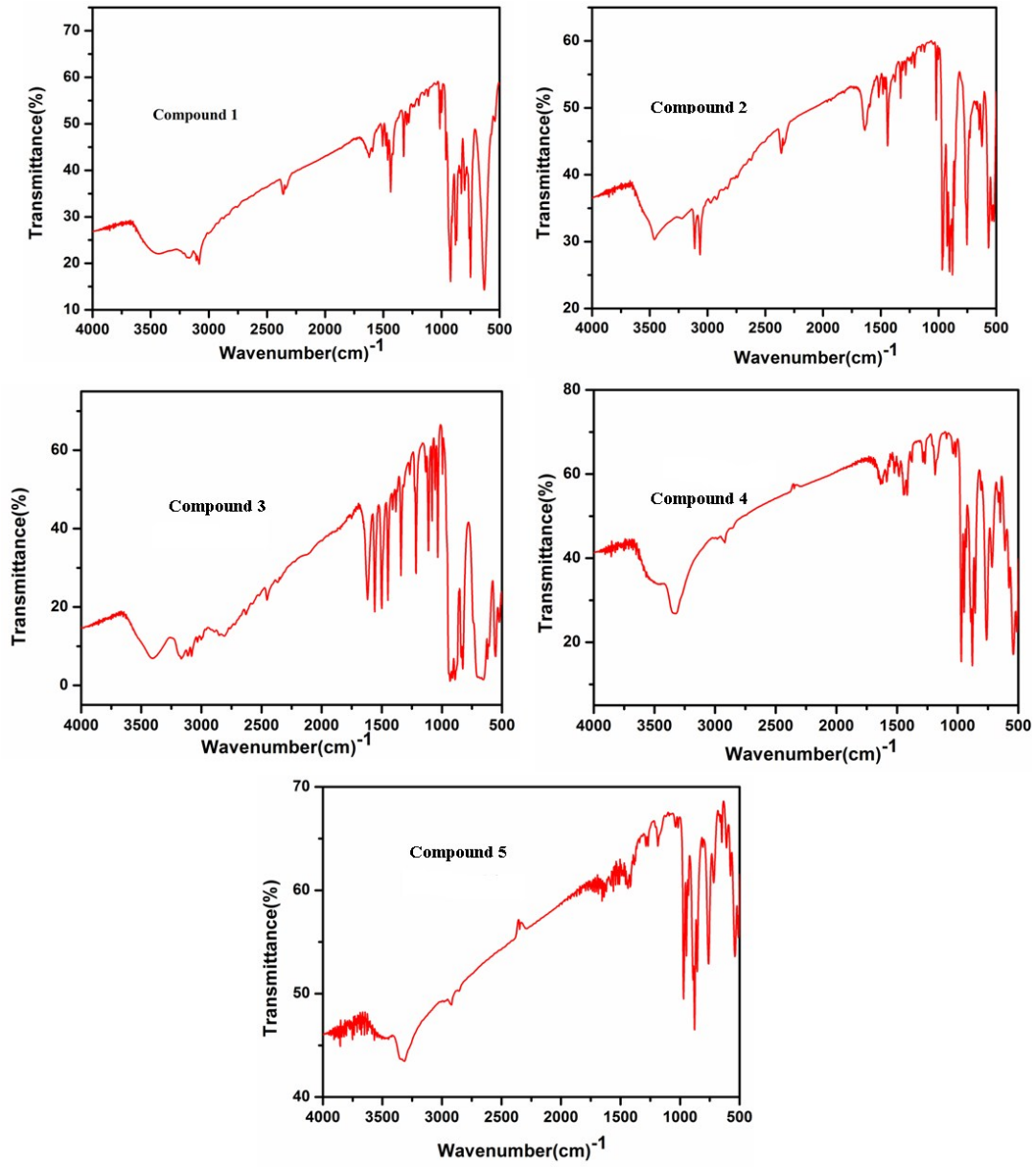

Fig. S5. The IR spectra of compounds **1**, **2**, **3**, **4** and **5**.

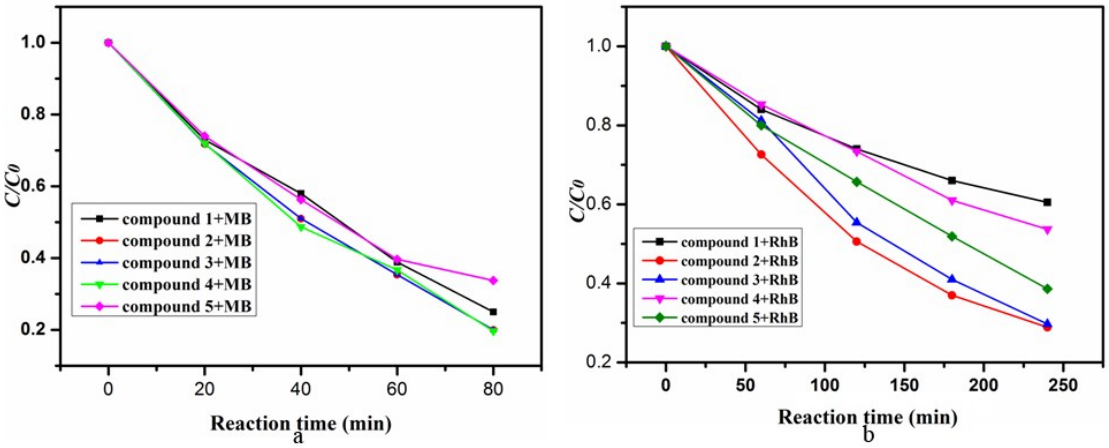

Fig. S6. Photocatalytic decomposition rates of MB (a) and RhB (b) solutions under UV irradiation with the use of compounds **1**, **2**, **3**, **4** and **5**.

Table S1. Selected bond distances (Å) and angles (°) for compounds **1**–**5**.

Compound **1**

N(1)-Cu(2)	2.052(6)	O(1W)-Cu(1)	1.924(5)
O(1W)-Cu(2)	1.943(5)	N(2)-Cu(1)	1.992(6)
Cu(2)-O(1W)#3	1.943(5)	Cu(2)-N(1)#3	1.943(5)
Cu(2)-N(1)#3	2.052(6)	Cu(2)-O(10)#3	2.359(5)
Cu(2)-O(10)	2.359(5)	Cu(1)-O(2W)	1.962(6)
Cu(1)-O(8)#4	1.982(5)	Cu(1)-O(12)	2.394(5)
Cu(1)-K(1)	3.579(2)	O(8)-Cu(1)#6	1.982(5)
C(1)-N(1)-Cu(2)	135.0(5)	N(2)-N(1)-Cu(2)	117.7(4)
Cu(1)-O(1W)-Cu(2)	120.0(2)	C(2)-N(2)-Cu(1)	132.6(5)
N(1)-N(2)-Cu(1)	119.3(4)	O(1W)#3-Cu(2)-O(1W)	179.999(1)
O(1W)#3-Cu(2)-N(1)	90.3(2)	O(1W)-Cu(2)-N(1)	89.7(2)
O(1W)#3-Cu(2)-N(1)#3	89.7(2)	O(1W)-Cu(2)-N(1)#3	90.3(2)
N(1)-Cu(2)-N(1)#3	179.999(1)	O(1W)#3-Cu(2)-O(10)#3	92.54(19)
O(1W)-Cu(2)-O(10)#3	87.46(19)	N(1)-Cu(2)-O(10)#3	90.2(2)
N(1)#3-Cu(2)-O(10)#3	89.8(2)	O(1W)#3-Cu(2)-O(10)	87.46(19)
O(1W)-Cu(2)-O(10)	92.54(19)	N(1)-Cu(2)-O(10)	89.8(2)
N(1)#3-Cu(2)-O(10)	90.2(2)	O(10)#3-Cu(2)-O(10)	180.000(1)

O(1W)-Cu(1)-O(2W)	89.9(3)	O(1W)-Cu(1)-O(12)	89.64(19)
O(2W)-Cu(1)-O(12)	91.7(2)	O(8)#4-Cu(1)-O(12)	103.42(19)
N(2)-Cu(1)-O(12)	86.9(2)	O(1W)-Cu(1)-K(1)	96.47(15)
O(2W)-Cu(1)-K(1)	6.9(2)	O(8)#4-Cu(1)-K(1)	83.30(14)
N(2)-Cu(1)-K(1)	171.51(17)	O(12)-Cu(1)-K(1)	89.33(14)
Mo(1)#1-O(8)-Cu(1)#6	146.6(3)	Cu(1)#6-O(8)-Mo(3)	100.54(18)
Mo(3)-O(10)-Cu(2)	169.2(3)	Mo(1)-O(12)-Cu(1)	170.2(3)
O(2W)-K(1)-Cu(1)	8.3(3)	O(5)#2-K(1)-Cu(1)	97.10(17)
K(1)#7-K(1)-Cu(1)	133.89(10)	O(7)#2-K(1)-Cu(1)	80.32(11)
Mo(4)#2-K(1)-Cu(1)	103.97(5)	Mo(2)#2-K(1)-Cu(1)	90.50(4)
K(1)-O(2W)-Cu(1)	164.8(5)		

Symmetry codes: #1 -x-1,-y+1,-z #2 -x,-y+1,-z #3 -x,-y+1,-z+1 #4 x+1,y,z #5 -x-1,-y+2,-z #6 x-1,y,z #7 -x,-y,-z

Compound **2**

Ag(1)-N(2)#2	2.221(4)	Ag(1)-N(1)	2.253(4)
Ag(1)-O(1)	2.320(3)	N(2)-Ag(1)#2	2.221(4)
N(2)#2-Ag(1)-N(1)	121.40(13)	N(2)#2-Ag(1)-O(1)	126.70(12)
N(1)-Ag(1)-O(1)	111.86(12)	Mo(4)-O(1)-Ag(1)	131.57(17)
C(1)-N(1)-Ag(1)	133.9(3)	N(2)-N(1)-Ag(1)	119.3(3)
C(2)-N(2)-Ag(1)#2	133.8(3)	N(1)-N(2)-Ag(1)#2	119.2(3)

Symmetry codes: 1 -x,-y,-z+1 #2 -x-1,-y,-z

Compound **3**

O(6)-Ag(1')#2	2.341(3)	O(6)-Ag(1)#2	2.493(4)
O(9)-Ag(1)	2.493(3)	N(1)-Ag(1')	2.347(5)
N(1)-Ag(1)	2.394(4)	N(1)-Ag(1)#2	2.491(4)
Ag(1)-Ag(1')	0.625(2)	Ag(1)-O(1W)	2.412(4)
Ag(1)-N(1)#2	2.491(4)	Ag(1)-O(6)#2	2.493(4)
Ag(1)-Ag(1)#2	2.656(4)	Ag(1)-Ag(1')#2	3.041(2)
Ag(1')-O(1W)	2.266(4)	Ag(1')-O(6)#2	2.341(3)

Ag(1')-Ag(1)#2	3.041(2)	Mo(2)-O(6)-Ag(1')#2	147.81(19)
Mo(2)-O(6)-Ag(1)#2	133.79(17)	Ag(1')#2-O(6)-Ag(1)#2	14.42(6)
Mo(1)-O(9)-Ag(1)	119.11(13)	Mo(2)-O(9)-Ag(1)	104.73(11)
Mo(3)-O(9)-Ag(1)	116.12(11)	C(1)-N(1)-Ag(1')	112.5(3)
N(2)-N(1)-Ag(1')	123.8(3)	C(1)-N(1)-Ag(1)	126.7(3)
N(2)-N(1)-Ag(1)	117.5(3)	Ag(1')-N(1)-Ag(1)	15.11(6)
C(1)-N(1)-Ag(1)#2	126.4(3)	N(2)-N(1)-Ag(1)#2	110.2(3)
Ag(1')-N(1)-Ag(1)#2	77.81(13)	Ag(1)-N(1)-Ag(1)#2	65.86(12)
Ag(1')-Ag(1)-N(1)	78.2(3)	Ag(1')-Ag(1)-O(1W)	69.2(3)
N(1)-Ag(1)-O(1W)	138.22(15)	Ag(1')-Ag(1)-N(1)#2	140.7(4)
N(1)-Ag(1)-N(1)#2	114.14(12)	O(1W)-Ag(1)-N(1)#2	107.63(15)
Ag(1')-Ag(1)-O(6)#2	68.9(3)	N(1)-Ag(1)-O(6)#2	91.56(13)
O(1W)-Ag(1)-O(6)#2	99.97(14)	N(1)#2-Ag(1)-O(6)#2	73.44(12)
Ag(1')-Ag(1)-O(9)	98.2(3)	N(1)-Ag(1)-O(9)	78.93(12)
O(1W)-Ag(1)-O(9)	80.58(13)	N(1)#2-Ag(1)-O(9)	120.45(13)
O(6)#2-Ag(1)-O(9)	165.44(12)	Ag(1')-Ag(1)-Ag(1)#2	122.8(4)
N(1)-Ag(1)-Ag(1)#2	58.83(12)	O(1W)-Ag(1)-Ag(1)#2	162.95(14)
N(1)#2-Ag(1)-Ag(1)#2	55.32(11)	O(6)#2-Ag(1)-Ag(1)#2	75.96(11)
O(9)-Ag(1)-Ag(1)#2	107.58(11)	Ag(1')-Ag(1)-Ag(1')#2	132.7(3)
N(1)-Ag(1)-Ag(1')#2	65.78(11)	O(1W)-Ag(1)-Ag(1')#2	155.28(12)
N(1)#2-Ag(1)-Ag(1')#2	48.99(11)	O(6)#2-Ag(1)-Ag(1')#2	82.08(9)
O(9)-Ag(1)-Ag(1')#2	103.58(8)	Ag(1)#2-Ag(1)-Ag(1')#2	9.95(6)
Ag(1)-Ag(1')-O(1W)	95.9(3)	Ag(1)-Ag(1')-O(6)#2	96.7(3)
O(1W)-Ag(1')-O(6)#2	109.24(15)	Ag(1)-Ag(1')-N(1)	86.7(3)
O(1W)-Ag(1')-N(1)	153.40(16)	O(6)#2-Ag(1')-N(1)	96.67(13)
Ag(1)-Ag(1')-Ag(1)#2	47.3(3)	O(1W)-Ag(1')-Ag(1)#2	141.23(15)
O(6)#2-Ag(1')-Ag(1)#2	70.86(9)	N(1)-Ag(1')-Ag(1)#2	53.20(11)
Ag(1')-O(1W)-Ag(1)	14.94(6)		

Symmetry codes: #1 -x,-y+1,-z+1 #2 -x+1,-y+1,-z+2

Compound **4**

Cu(1)-O(3)	1.948(10)	Cu(1)-N(1)#2	1.956(14)
Cu(1)-O(7)	1.953(10)	Cu(1)-N(3)	1.955(14)
N(1)-Cu(1)#3	1.956(14)	O(3)-Cu(1)-N(1)#2	165.8(5)
O(3)-Cu(1)-O(7)	86.8(4)	N(1)#2-Cu(1)-O(7)	93.1(5)
O(3)-Cu(1)-N(3)	90.2(5)	N(1)#2-Cu(1)-N(3)	93.1(6)
O(7)-Cu(1)-N(3)	166.2(5)	C(3)-N(1)-Cu(1)#3	133.4(13)
N(2)-N(1)-Cu(1)#3	121.1(12)	Mo(2)-O(3)-Cu(1)	154.4(6)
C(9)-N(3)-Cu(1)	131.7(11)	N(4)-N(3)-Cu(1)	121.0(11)
Mo(3)-O(7)-Cu(1)	153.9(6)		

Symmetry codes: #1 -x-1,-y+1,-z+1 #2 x-1,y,z #3 x+1,y,z #4 -x,-y+1,-z+1

Compound **5**

Ag(2)-N(1)	2.155(5)	Ag(2)-N(4)#1	2.160(6)
Ag(2)-O(11)	2.511(5)	Ag(1)-N(3)	2.212(5)
Ag(1)- O(11)	2.670(5)	Ag(1)- O(6)	2.819(5)
Ag(1)- O(7)	2.801(6)	Ag(1)- O(5)	2.772(6)
Ag(1)-N(2)#3	2.208(5)	N(4)-Ag(2)#4	2.160(6)
N(2)-Ag(1)#3	2.208(5)	N(1)-Ag(2)-O(11)	89.59(18)
N(1)-Ag(2)-N(4)#1	160.8(2)	N(4)#1-Ag(2)-O(11)	103.70(18)
N(3)-Ag(1)-N(2)#3	165.8(2)	C(1)-N(2)-Ag(1)#3	127.7(5)
N(1)-N(2)-Ag(1)#3	124.3(4)	C(7)-N(3)-Ag(1)	124.3(4)
N(4)-N(3)-Ag(1)	127.6(4)	C(2)-N(1)-Ag(2)	125.3(5)
N(2)-N(1)-Ag(2)	126.9(4)	Mo(1)-O(11)-Ag(2)	134.2(3)
C(8)-N(4)-Ag(2)#4	124.8(4)	N(3)-N(4)-Ag(2)#4	128.3(4)

Symmetry codes: #1 x,y-1,z #2 -x+1,-y-2,-z+1 #3 -x+1,-y,-z+2 #4 x,y+1,z