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Three β-Octamolybdate-based Supramolecular Hybrids Constructed from a Bis-imidazolyl-bis-amide Ligand: Fast and Selective Adsorption Activities of Organic Dyes

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Table S1 Selected hydrogen bonding geometry (Å, °) for compound **1**.

D–H···A	D–H / Å	H···A / Å	D···A / Å	D–H···A / °
O(1)–H(2WA)···O(2W)	0.85	2.20	3.021	160
N(4)–H(4C)···O(2W)	0.86	2.16	2.903	145
N(6)–H(6B)···O(8)	0.86	2.19	3.009	160

Table S2 Selected hydrogen bonding geometry (Å, °) for compound **3**.

D–H···A	D–H / Å	H···A / Å	D···A / Å	D–H···A / °
N(10)–H(6C)···O(24)	0.86	2.10	2.949	169
N(11)–H(5C)···O(32)	0.86	2.05	2.910	176
N(9)–H(9A)···O(19)	0.86	2.13	2.965	162

Table S3 Selected bond distances (Å) and angles (°) for compounds **1**–**3**.

Compound 1			
Mo(1)-O(9)	1.696(2)	Mo(2)-O(13)	1.918(2)
Mo(1)-O(8)	1.759(2)	Mo(2)-O(8)	2.264(2)
Mo(1)-O(16)#1	1.926(2)	Mo(2)-O(11)#1	2.513(2)
Mo(1)-O(15)	1.962(2)	O(16)-Mo(1)#1	1.926(2)
Mo(1)-O(11)	2.109(2)	O(16)-Mo(3)	2.014(2)
Mo(1)-O(11)#1	2.371(2)	O(16)-Mo(4)	2.397(2)
Mo(1)-Mo(4)	3.2064(4)	Mo(3)-O(5)	1.692(3)
Co(1)-N(2)	2.049(3)	Mo(3)-O(4)	1.706(3)
Co(1)-N(1)	2.099(3)	Mo(3)-O(13)	1.886(2)
Co(1)-O(1W)	2.125(3)	Mo(3)-O(11)#1	2.371(2)
Co(1)-O(3)	2.128(3)	Mo(4)-O(10)	1.694(3)
Co(1)-O(2)	2.132(2)	Mo(4)-O(14)	1.713(3)
Co(1)-O(1)	2.189(3)	Mo(4)-O(6)#1	1.897(2)
O(15)-Mo(4)	1.998(2)	Mo(4)-O(11)	2.286(2)
O(15)-Mo(3)	2.311(2)	O(6)-Mo(4)#1	1.897(2)
Mo(2)-O(7)	1.682(3)	O(11)-Mo(3)#1	2.371(2)

Mo(2)-O(2)	1.727(2)	O(11)-Mo(1)#1	2.371(2)
Mo(2)-O(6)	1.910(2)	O(11)-Mo(2)#1	2.513(2)
N(2)-Co(1)-N(1)	176.77(12)	O(3)-Co(1)-O(2)	90.67(10)
N(2)-Co(1)-O(1W)	90.19(12)	N(2)-Co(1)-O(1)	77.49(11)
N(1)-Co(1)-O(1W)	87.68(12)	N(1)-Co(1)-O(1)	105.04(11)
N(2)-Co(1)-O(3)	103.94(11)	O(1W)-Co(1)-O(1)	92.85(10)
N(1)-Co(1)-O(3)	78.31(11)	O(3)-Co(1)-O(1)	87.77(10)
O(1W)-Co(1)-O(3)	165.63(10)	O(2)-Co(1)-O(1)	165.13(10)
N(2)-Co(1)-O(2)	88.56(11)		
N(1)-Co(1)-O(2)	89.09(11)		
O(1W)-Co(1)-O(2)	92.31(10)		

Symmetry codes for **1**: #1 – x + 1, – y + 1, – z – 1.

Compound 2

Mo(1)-O(11)	1.693(4)	Mo(2)-O(14)	2.520(3)
Mo(1)-O(12)	1.764(3)	Mo(3)-O(8)	1.695(4)
Mo(1)-O(20)#1	1.926(3)	Mo(3)-O(7)	1.706(4)
Mo(1)-O(13)	1.964(4)	Mo(3)-O(15)	1.892(4)
Mo(1)-O(14)#1	2.109(3)	Mo(3)-O(20)	2.018(3)
Mo(1)-O(14)	2.372(3)	Mo(3)-O(13)	2.312(3)
Mo(1)-Mo(4)	3.2133(7)	Mo(3)-O(14)	2.355(3)
Zn(1)-N(1)	2.017(4)	Mo(4)-O(10)	1.693(4)
Zn(1)-N(3)	2.073(4)	Mo(4)-O(9)	1.707(4)
Zn(1)-O(1W)	2.149(4)	Mo(4)-O(17)#1	1.894(4)
Zn(1)-O(1)	2.173(4)	Mo(4)-O(13)	2.001(3)
Zn(1)-O(6)	2.204(4)	Mo(4)-O(14)#1	2.299(3)
Zn(1)-O(2)	2.217(4)	Mo(4)-O(20)	2.405(3)
Mo(2)-O(16)	1.689(4)	O(14)-Mo(1)#1	2.109(3)
Mo(2)-O(6)	1.724(4)	O(14)-Mo(4)#1	2.299(3)
Mo(2)-O(17)	1.910(4)	O(17)-Mo(4)#1	1.894(4)
Mo(2)-O(15)	1.919(3)	O(20)-Mo(1)#1	1.926(3)
Mo(2)-O(12)	2.262(3)	N(3)-Zn(1)-O(2)	106.01(16)
N(1)-Zn(1)-N(3)	176.03(18)	O(1W)-Zn(1)-O(2)	94.11(15)
N(1)-Zn(1)-O(1W)	90.76(16)	O(1)-Zn(1)-O(2)	88.44(15)
N(3)-Zn(1)-O(1W)	88.30(16)	O(6)-Zn(1)-O(2)	163.25(13)
N(1)-Zn(1)-O(1)	102.33(16)		
N(3)-Zn(1)-O(1)	78.66(16)		
O(1W)-Zn(1)-O(1)	166.91(14)		
N(1)-Zn(1)-O(6)	86.41(15)		
N(3)-Zn(1)-O(6)	89.77(16)		
O(1W)-Zn(1)-O(6)	91.91(14)		
O(1)-Zn(1)-O(6)	89.23(15)		
N(1)-Zn(1)-O(2)	77.90(15)		

Symmetry codes for **2**: #1 – x, – y + 1, – z.

Compound 3

Mo(1)-O(18)	1.692(5)	Mo(4)-Mo(3)#2	3.2083(9)
Mo(1)-O(17)	1.753(4)	Mo(5)-O(32)	1.692(5)
Mo(1)-O(21)#1	1.946(4)	Mo(5)-O(16)	1.695(5)
Mo(1)-O(5)	1.950(5)	Mo(5)-O(12)	1.895(5)
Mo(1)-O(15)	2.146(4)	Mo(5)-O(5)	2.005(4)
Mo(1)-O(15)#1	2.403(4)	Mo(5)-O(15)	2.315(4)
Mo(1)-Mo(2)#1	3.2108(9)	Mo(5)-O(21)	2.360(4)
Cu(1)-N(1)	1.902(6)	Mo(6)-O(27)	1.688(5)
Cu(1)-N(2)	1.918(6)	Mo(6)-O(28)	1.699(5)
Cu(1)-O(1)	1.965(5)	Mo(6)-O(26)	1.875(5)
Cu(1)-O(2)	1.967(5)	Mo(6)-O(29)	2.007(4)
Mo(2)-O(13)	1.695(5)	Mo(6)-O(30)	2.393(5)
Mo(2)-O(9)	1.719(5)	Mo(6)-O(25)	2.395(5)
Mo(2)-O(10)	1.888(4)	Mo(7)-O(8)	1.682(5)
Mo(2)-O(21)	1.985(4)	Mo(7)-O(7)	1.707(5)
Mo(2)-O(15)#1	2.315(4)	Mo(7)-O(12)#1	1.933(5)
Mo(2)-O(5)	2.347(5)	Mo(7)-O(10)	1.934(5)
Mo(2)-Mo(1)#1	3.2108(9)	Mo(7)-O(17)	2.296(5)
Cu(2)-N(5)	1.951(6)	Mo(7)-O(15)#1	2.492(4)
Cu(2)-N(6)	1.958(6)	Mo(8)-O(14)	1.690(5)
Cu(2)-O(4)	1.980(5)	Mo(8)-O(20)	1.694(6)
Cu(2)-O(3)	1.981(5)	Mo(8)-O(26)#2	1.905(5)
Cu(2)-O(5W)	2.357(6)	Mo(8)-O(23)	1.964(5)
Mo(3)-O(11)	1.691(5)	Mo(8)-O(19)	2.319(5)
Mo(3)-O(19)	1.765(4)	Mo(8)-O(30)#2	2.474(4)
Mo(3)-O(25)#2	1.935(4)	O(12)-Mo(7)#1	1.933(5)
Mo(3)-O(29)	1.953(4)	O(15)-Mo(2)#1	2.315(4)
Mo(3)-O(30)	2.123(4)	O(15)-Mo(1)#1	2.403(4)
Mo(3)-O(30)#2	2.393(5)	O(15)-Mo(7)#1	2.492(4)
Mo(3)-Mo(4)#2	3.2082(9)	O(21)-Mo(1)#1	1.946(4)
Mo(4)-O(31)	1.706(5)	O(25)-Mo(3)#2	1.935(4)
Mo(4)-O(24)	1.715(5)	O(26)-Mo(8)#2	1.905(5)
Mo(4)-O(23)	1.877(5)	O(30)-Mo(4)#2	2.310(5)
Mo(4)-O(25)	1.989(4)	O(30)-Mo(3)#2	2.393(5)
Mo(4)-O(30)#2	2.310(5)	O(30)-Mo(8)#2	2.474(4)
Mo(4)-O(29)	2.337(5)	O(4)-Cu(2)-O(3)	179.4(3)
N(1)-Cu(1)-N(2)	176.2(3)	N(5)-Cu(2)-O(5W)	103.5(2)
N(1)-Cu(1)-O(1)	83.4(2)	N(6)-Cu(2)-O(5W)	89.3(3)
N(2)-Cu(1)-O(1)	98.6(2)	O(4)-Cu(2)-O(5W)	86.3(2)
N(1)-Cu(1)-O(2)	94.0(2)	O(3)-Cu(2)-O(5W)	94.3(2)
N(2)-Cu(1)-O(2)	83.8(2)		
O(1)-Cu(1)-O(2)	176.1(2)		
N(5)-Cu(2)-N(6)	167.2(3)		
N(5)-Cu(2)-O(4)	96.7(2)		

N(6)-Cu(2)-O(4)	83.1(2)
N(5)-Cu(2)-O(3)	83.2(2)
N(6)-Cu(2)-O(3)	96.8(2)

Symmetry codes for **3**: #1 – x, – y + 1, – z + 1; #2 – x + 1, – y + 1, – z.

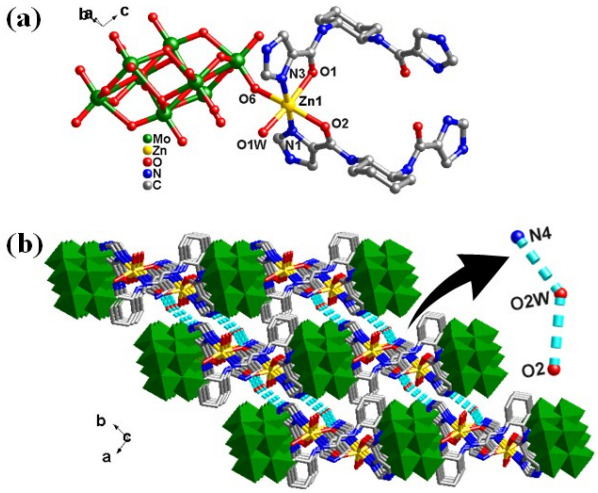

Fig.S1 (a) Stick/ball view of the asymmetric unit of **2**. The hydrogen atoms are omitted for clarity. (b) View of the 3D supramolecular structure of **2**.

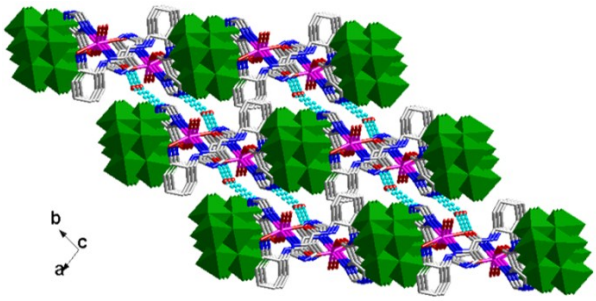

Fig.S2 View of the 3D supramolecular structure of **1.**

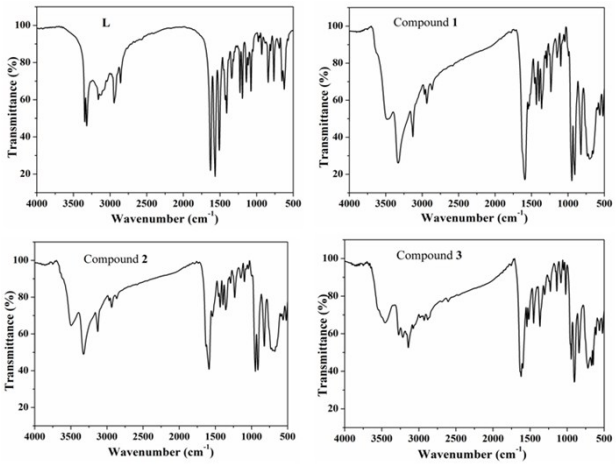

Fig.S3 The IR spectra of compounds **1**–**3** and **L**.

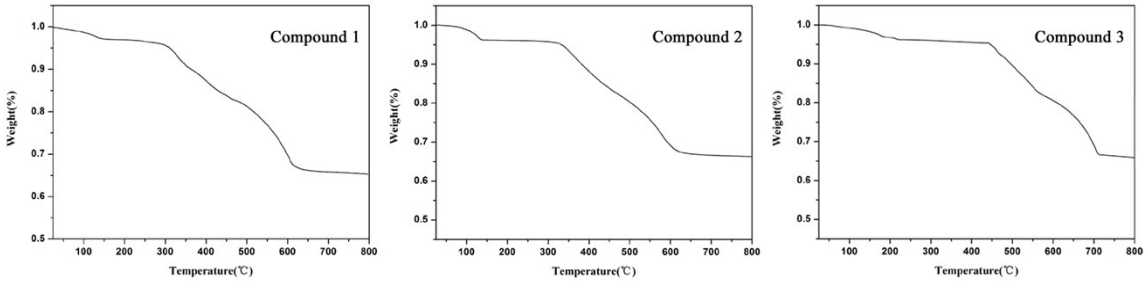

Fig.S4 The thermogravimetric (TG) curves of compounds **1**−**3**.

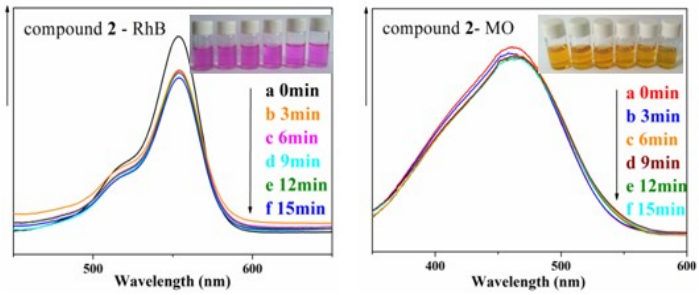

Fig.S5 The UV absorption curves of RhB and MO with **2**.

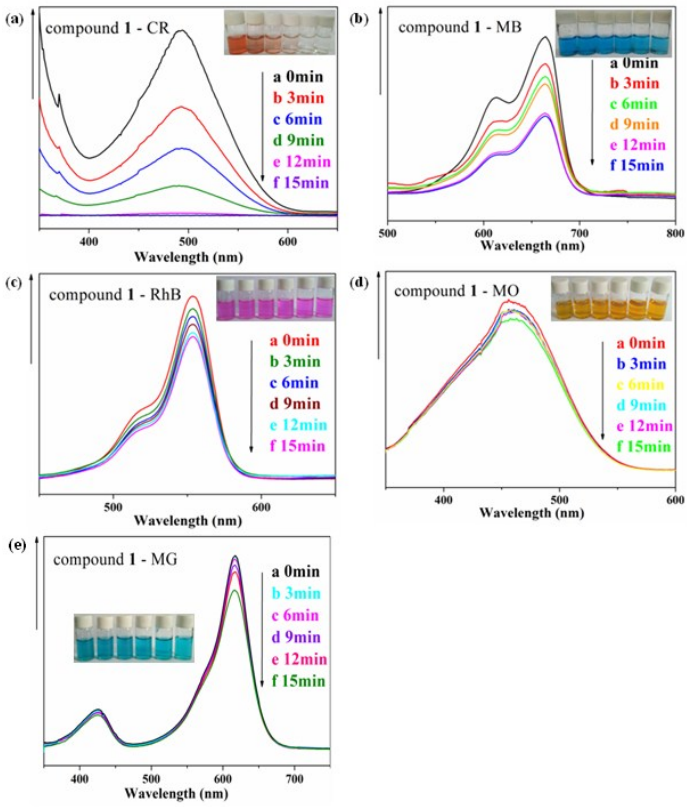

Fig.S6 (a-e) The UV absorption curves of CR, MB, RhB, MO and MG with **1**.

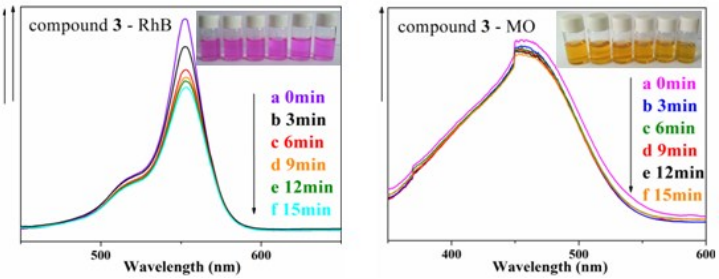

Fig.S7 The UV absorption curves of RhB and MO with **3**; The inserted photographs show the change of solution colors with the increase of time.