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Template-Assisted Self-Assembly: Design and Synthesis of the $[MoOS_3Cu_3]^+$ based supramolecular polymeric clusters

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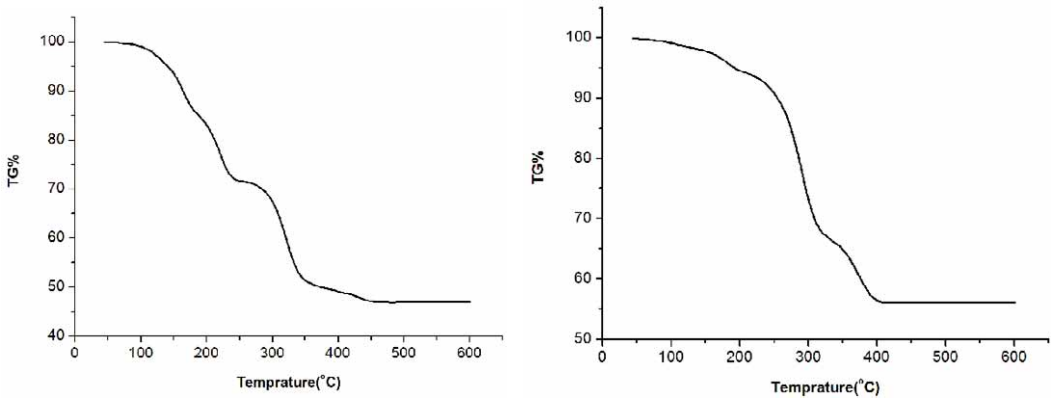
Table S1 Selected bond distances (Å) and angles (deg) for the polymers 1–4[a]

1					
I(1)-Cu(2)	2.5524(9)	Mo(1)-O(1)	1.706(4)	Mo(1)-S(1)	2.2518(16)
Mo(1)-Cu(1)	2.7171(9)	Cu(1)-N(4)^1	2.046(5)	Cu(1)-S(2)	2.2835(17)
Cu(2)-S(1)	2.3049(15)	Cu(2)-N(2)^2	2.176(4)		
O(1)-Mo(1)-S(1)	111.21(17)	S(1)-Mo(1)-S(3)	107.48(6)	Cu(3)-Mo(1)-Cu(2)	92.02(2)
O(1)-Mo(1)-Cu(1)	127.51(17)	S(1)-Cu(1)-Mo(1)	52.50(4)	N(1)-Cu(1)-Mo(1)	121.27(15)
N(2)-Cu(2)-I(1)	103.32(14)	N(4)-Cu(1)-S(1)	110.52(14)	N(4)-Cu(1)-N(1)	109.5(2)
2					
Mo(1)-O(1)	1.704(6)	Mo(1)-S(1)	2.261(2)	Mo(1)-Cu(1)	2.7099(13)
I(1)-Cu(1)	2.4266(15)	S(1)-Cu(1)	2.263(2)	Cu(1)-N(1)	2.175(6)
Cu(3)-N(5)#1	2.050(7)	Cu(3)-N(2)#2	2.070(7)	N(2)-Cu(3)#3	2.070(7)
O(1)-Mo(1)-S(1)	110.3(3)	S(1)-Mo(1)-S(2)	108.97(8)	O(1)-Mo(1)-Cu(2)	125.4(2)
S(1)-Mo(1)-Cu(2)	54.79(6)	S(3)-Mo(1)-Cu(2)	123.39(6)	Mo(1)-S(1)-Cu(1)	73.60(7)
Cu(2)-Mo(1)-Cu(1)	91.51(4)	N(1)-Cu(1)-S(1)	110.0(2)	N(1)-Cu(1)-Mo(1)	109.5(2)
N(4)-Cu(2)-N(3)	109.7(3)				
3					
Mo(1)-Cu(1)	2.6806(8)	Mo(1)-S(1)	2.2676(15)	Mo(1)-O(1)	1.699(4)
Br(1)-Cu(3)	2.4278(9)	Cu(1)-S(1)	2.2921(16)	Cu(1)-N(1)	2.016(4)
Cu(2)-N(2)^1	2.065(4)	Cu(3)-N(5)^2	2.182(4)		
Cu(1)-Mo(1)-Cu(2)	88.08(3)	S(1)-Mo(1)-Cu(1)	54.42(4)	S(1)-Mo(1)-S(2)	108.36(6)
S(2)-Mo(1)-Cu(3)	126.28(4)	O(1)-Mo(1)-Cu(1)	125.79(16)	O(1)-Mo(1)-S(1)	110.90(17)
S(1)-Cu(1)-Mo(1)	53.57(4)	S(2)-Cu(1)-S(1)	107.52(6)	N(2)^1-Cu(2)-Mo(1)	128.83(14)
N(2)^1-Cu(2)-S(3)	110.02(14)	Br(1)-Cu(3)-Mo(1)	146.90(3)	N(5)^2-Cu(3)-Br(1)	102.65(13)
4					
Mo(1)-O(1)	1.710(4)	Mo(1)-S(1)	2.2618(19)	Mo(1)-Cu(1)	2.6834(10)
Cu(1)-N(1)	2.048(5)	Cu(1)-S(1)	2.2842(18)	Cu(3)-N(5)#1	2.043(5)
Cu(3)-N(2)#2	2.107(5)				
O(1)-Mo(1)-S(1)	110.7(2)	S(1)-Mo(1)-S(3)	108.16(6)	O(1)-Mo(1)-Cu(3)	129.56(19)
S(1)-Mo(1)-Cu(3)	119.78(5)	S(2)-Mo(1)-Cu(3)	54.46(5)	Cu(1)-Mo(1)-Cu(2)	89.43(3)
N(1)-Cu(1)-N(3)	105.94(18)	N(1)-Cu(1)-S(3)	116.14(15)	N(1)-Cu(1)-Mo(1)	134.23(13)
N(5)#1-Cu(3)-N(2)#2	99.8(2)	Mo(1)-S(1)-Cu(1)	72.35(6)	Cu(1)-S(1)-Cu(2)	111.65(7)

Cu(2)-S(2)-Cu(3)	106.78(7)	Cu(3)-S(3)-Mo(1)	72.25(5)

[a] Symmetry transformations used to generate equivalent atoms for **1**: [1]1-X, +Y, 1/2-Z; [2]1/2-X, -1/2+Y, -1/2-Z. For **2**: #1: -x+1, y, -z+3/2. #2: -x+1/2, y+1/2, -z+1/2. #3: -x+1/2, y-1/2, -z+1/2. For **3**: [1]-X, +Y, 1/2-Z; [2]1/2-X, -1/2+Y, 3/2-Z. For **4**: #1: x, -y+2, z-1/2. #2: -x+1/2, -y+1/2, -z.



S1 S2

Fig. S1： The TG curve of compound **1**. S2: The TG curve of compound **2.**