Supporting Information

Modulating energetic performance through decorating the nitrogen-rich ligands in high-energy MOFs

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Contents

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Table S1 Selected crystallographic data and structural refinement for compounds **1** and **2**

	1	**2**
Empirical formula	$C_3H_4AgN_4O_2$	$C_3H_4AgN_5O_2$
Formula weight	235.97	249.98
Temperature/K	293(2)	293(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a (Å)	8.8458(15)	4.2779(9)
b (Å)	6.0291(10)	10.937(2)
c (Å)	10.7271(18)	14.054(3)
α (°)	90	90
β (°)	104.815	105.837(8)
γ (°)	90	90
V (Å^3)	553.08	632.6(2)
Z	4	4
D (Mg/m^3)	2.834	2.625
μ (mm^{-1})	3.573	3.136
Unique reflections	1364	1113
Observed reflections	1539	10565
R_{int}	0.0771	0.0690
R_1 [$I > 2\sigma(I)$]	R1 = 0.0562, wR2 = 0.1342	R_1 = 0.1073, wR_2 = 0.2834
wR_2 (all data)	R1 = 0.0636, wR2 = 0.1397	R_1 = 0.1143, wR_2 = 0.2886

Table S2 Selected bond lengths [Å] and bond angles [°] for **1** and **2**

1		**2**	
Ag(1)-N(2)	2.199(7)	Ag(1)-O(1)#5	2.265(13)
Ag(1)-N(3)#1	2.219(7)	Ag(1)-N(1)	2.200(14)
Ag(1)-O(1)#2	2.568(6)	Ag(1)-N(2)#7	2.322(14)
Ag(1)-N(4)#3	2.370(7)	O(1)-Ag(1)#2	2.265(13)
N(2)-Ag(1)-N(3)#1	137.3(2)	N(2)-Ag(1)#7	2.322(14)
N(2)-Ag(1)-O(1)#2	90.3(2)	O(1)#1-Ag(1)-N(2)#7	104.5(5)
N(2)-Ag(1)-N(4)#3	113.4(2)	N(1)-Ag(1)-O(1)#5	138.1(5)
N(3)#1-Ag(1)-O(1)#2	113.1(2)	N(1)-Ag(1)-N(2)#7	117.3(5)
N(3)#1-Ag(1)-N(4)#3	104.4(2)	C(3)-O(1)-Ag(1)#2	111.7(11)
N(4)#3-Ag(1)-O(1)#2	83.9(2)	N(2)-N(1)-Ag(1)	121.9(10)
N(3)-N(2)-Ag(1)	122.0(5)	C(1)-N(1)-Ag(1)	130.3(12)
N(1)-N(2)-Ag(1)	132.1(5)	N(1)-N(2)-Ag(1)#7	119.9(10)
N(2)-N(3)-Ag(1)#4	122.6(5)	N(3)-N(2)-Ag(1)#7	128.6(11)
N(4)-N(3)-Ag(1)#4	122.6(5)	C(1)-N(4)-C(2)	127.9(14)
C(1)-O(1)-Ag(1)#5	2.370(7)	O(1)- C(3)-C(2)	117.9(14)
N(3)-N(4)-Ag(1)#6	127.4(5)	N(2)-N(3)-N(4)	105.2(14)
C(3)-N(4)-Ag(1)#6	122.9(5)	N(1)-C(1)-N(4)	106.0(14)

#1 -x+1, y+1/2, -z+1/2 ; #2 x, -y+3/2, z-1/2 ; #3 x, -y+1/2, z-1/2; #4 -x+1, y-1/2, -z+1/2 ; #5 x, -y+3/2, z+1/2;

#6 x, -y+1/2, z+1/2 ; #7 - x, 1- y, 1-z

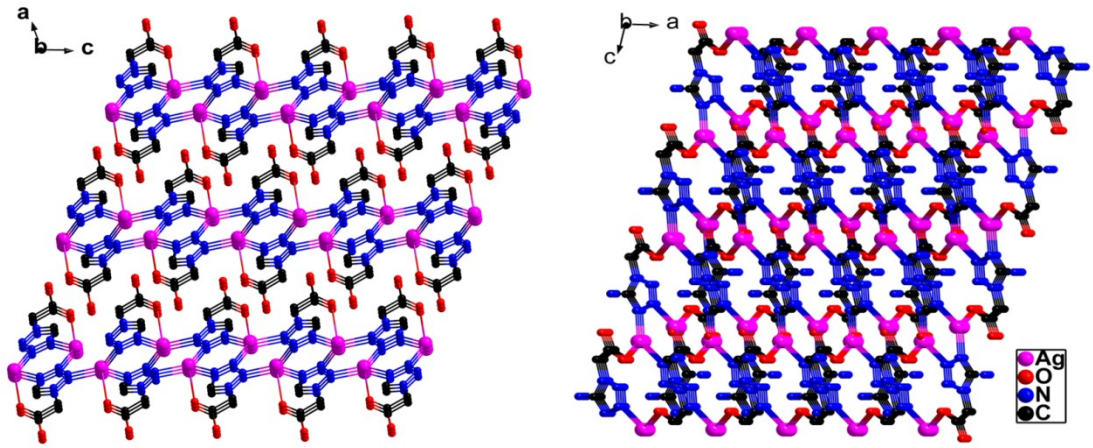

Fig. S1. 3D supramolecular network formed by several 2D layers in **1** (left) and **2** (right). (Hydrogen atoms are omitted for clarity).

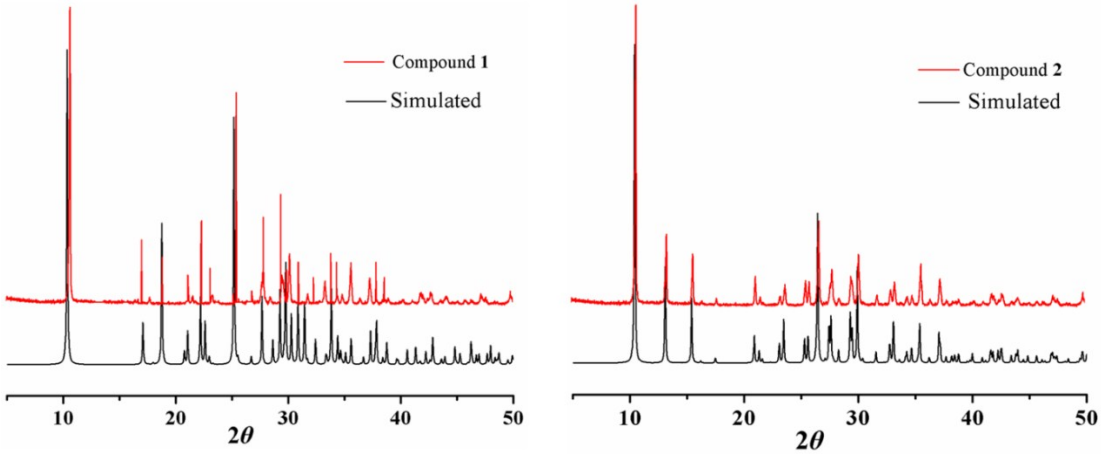

Fig. S2. PXRD patterns for compounds **1** (left) and **2** (right).

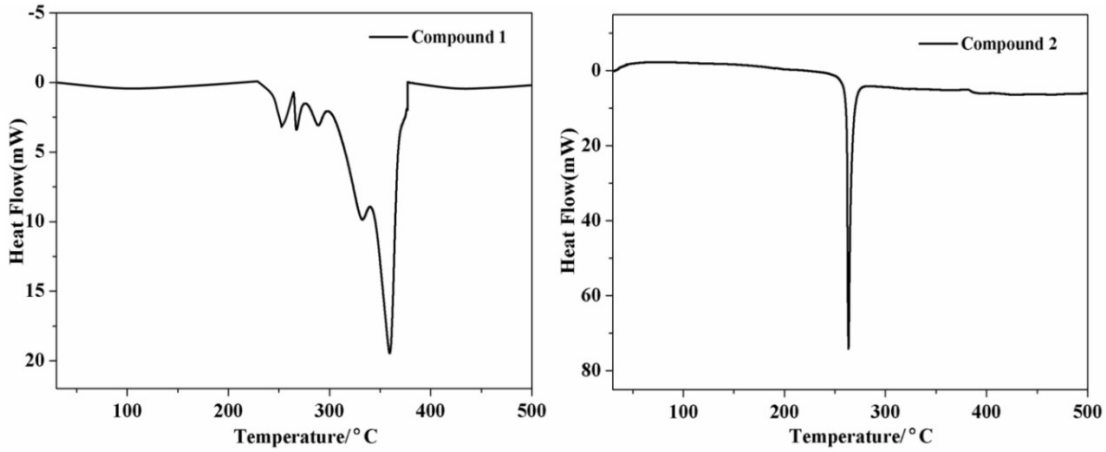

Fig. S3. DSC curves of **1** (left) and **2** (right).