Electronic Supplementary Information (ESI)

Ag(I) and Zn(II) coordination polymers with a bulky naphthalene-based di-carboxyl tecton and different 4,4'-bipyridyl-like bridging co-ligands: structural regulation and properties

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Dalton Trans.

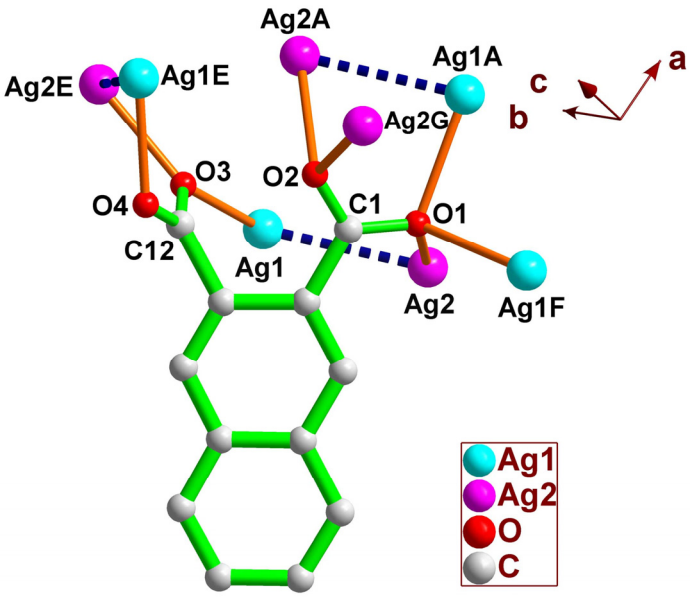


Fig. S1 A portion view of **1** showing the coordination mode of **ndc** and Ag1···Ag2 contact (dashed line) (A = –*x* + 1, –*y* + 2, –*z* + 1; E = *x*, –*y* + 3/2, *z* – 1/2; F = *x*, *y* + 1, *z*; G = *x*, – *y* + 5/2, *z* – 1/2).

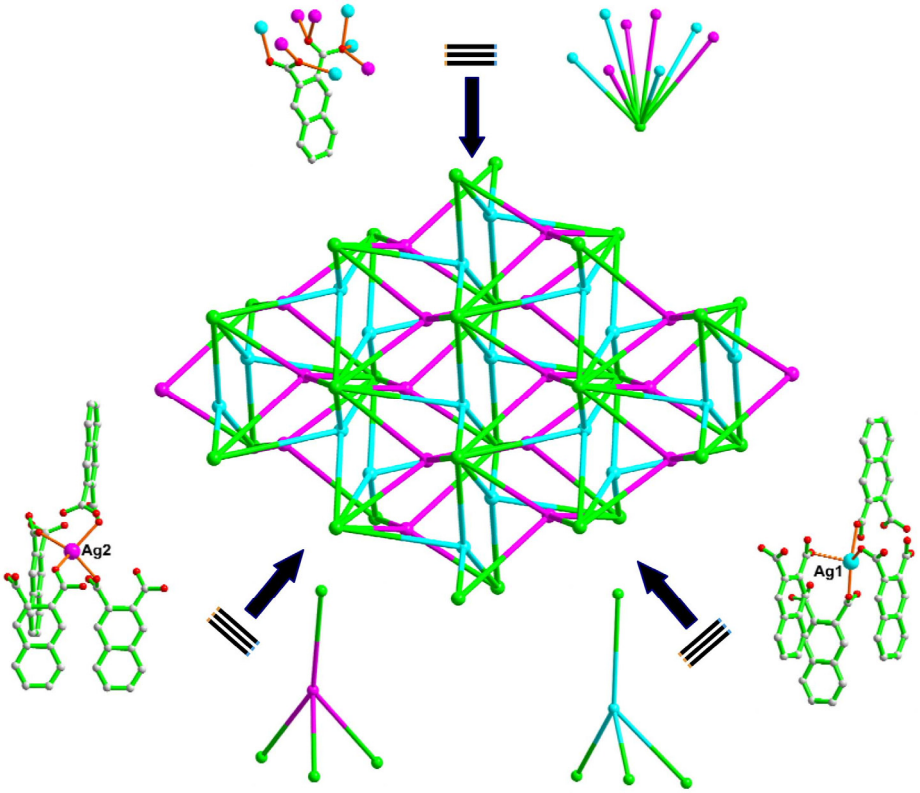


Fig. S2 A schematic representation of the (4,8)-connected 2-D topological network in **1** with the Schläfli symbol of $(4^6)_2(4^{16}.6^{11}.8)$, around which the detailed illustration of the connectivity of Ag(I) centers and **ndc** ligands is shown (cyan spheres for Ag1, pink spheres for Ag2, and green spheres for **ndc**).

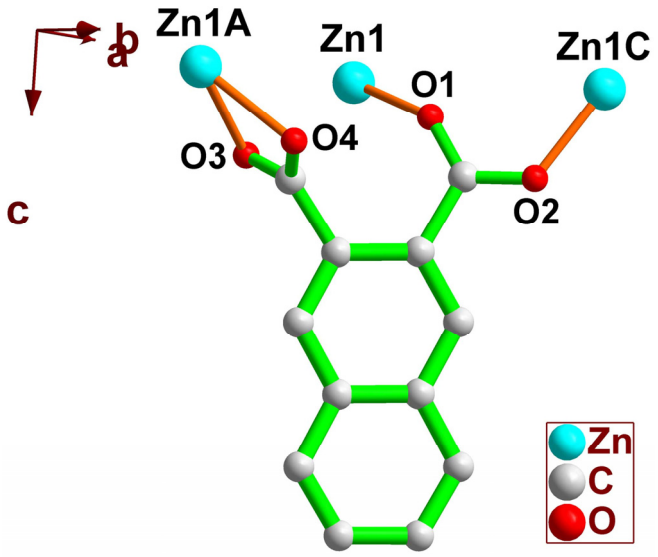


Fig. S3 A portion view of **2** showing the coordination mode of **ndc** (A = –*x*, –*y*, –*z* + 1; C = –*x* + 1/2, *y* + 1/2, *z*).

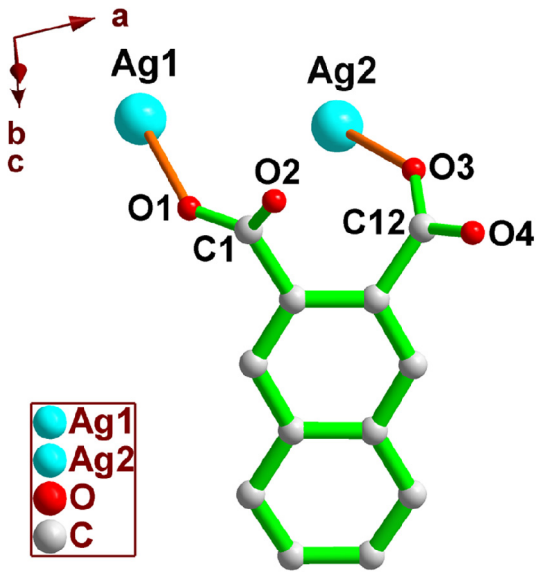


Fig. S4 A portion view of **3** showing the coordination mode of **ndc**.

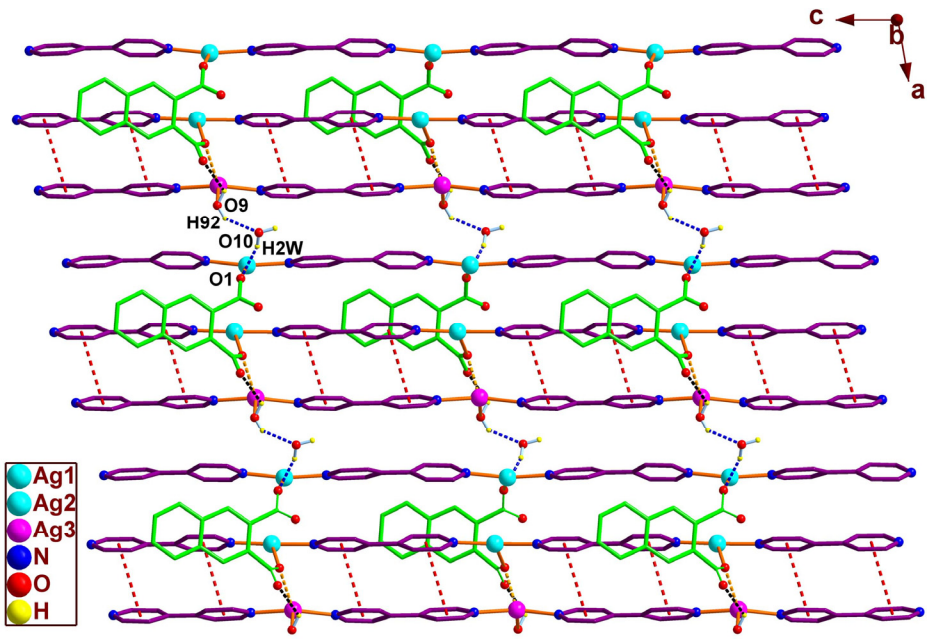


Fig. S5 View of the 2-D layered network along the (010) plane in **3**, formed by interchain O–H···O interactions (blue dashed lines) between the lattice water molecules and chains **A** and **B**.

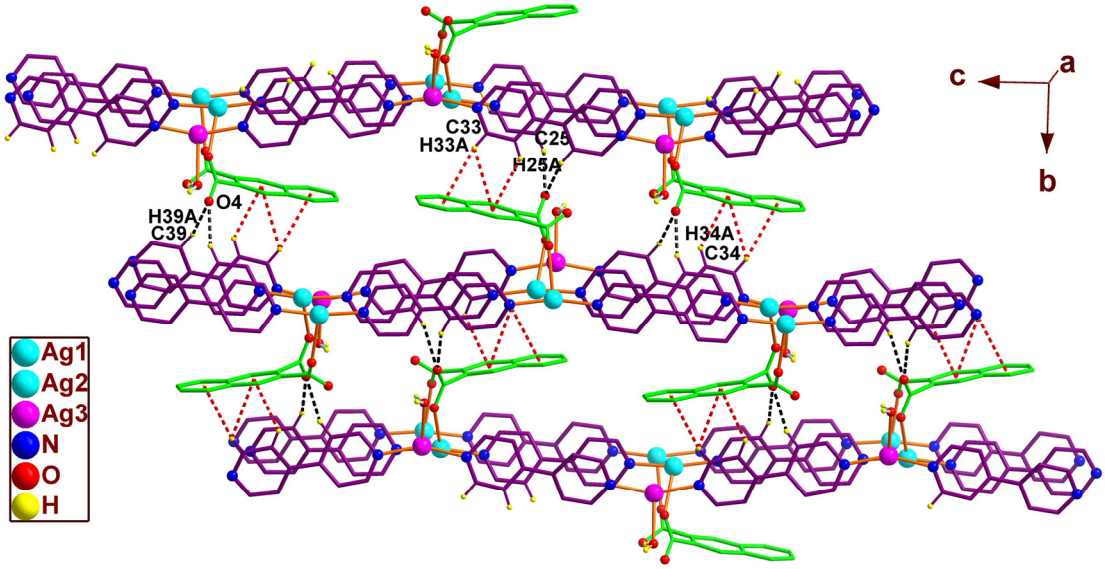


Fig. S6 View of another 2-D layer in **3**, running parallel to the (100) plane, formed by interchain C–H···O (black dashed lines) and C–H···π (red dashed lines) interactions between **ndc** and 4bpy ligands.

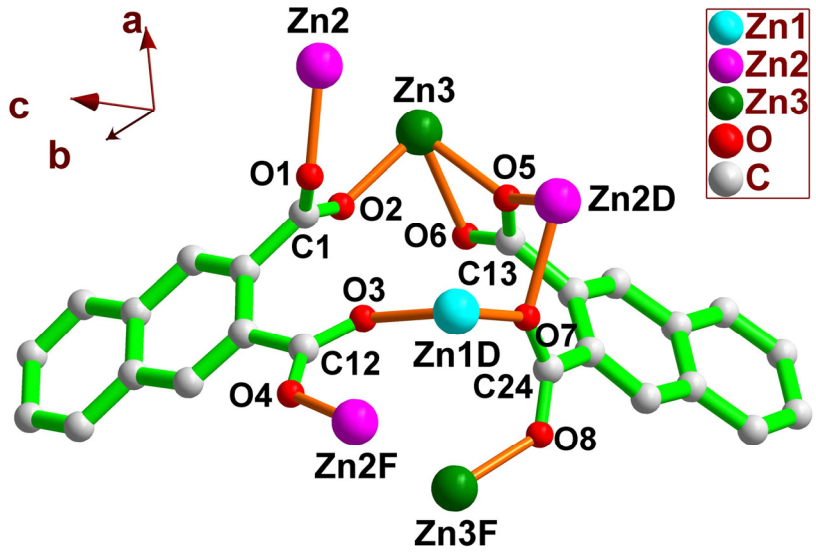


Fig. S7 A portion view of **4** showing the coordination mode of **ndc** (D = –*x*, –*y* + 2, –*z*; F = *x* + 1, *y*, *z*).

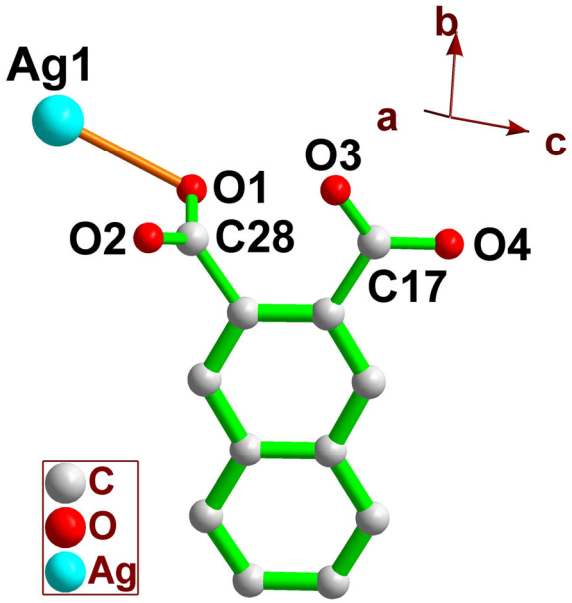


Fig. S8 A portion view of **5** showing the coordination mode of **ndc**.

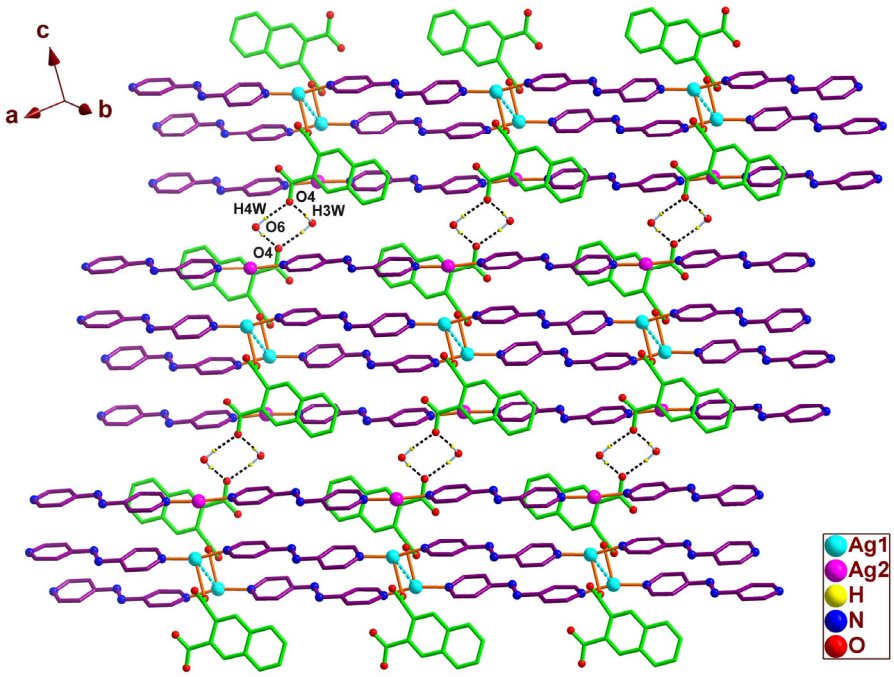


Fig. S9 View of the 2-D layered net in **5**, running parallel to the (111) plane, formed by interchain O–H···O interactions (blue dashed lines) between the lattice water molecules and chain **A**.

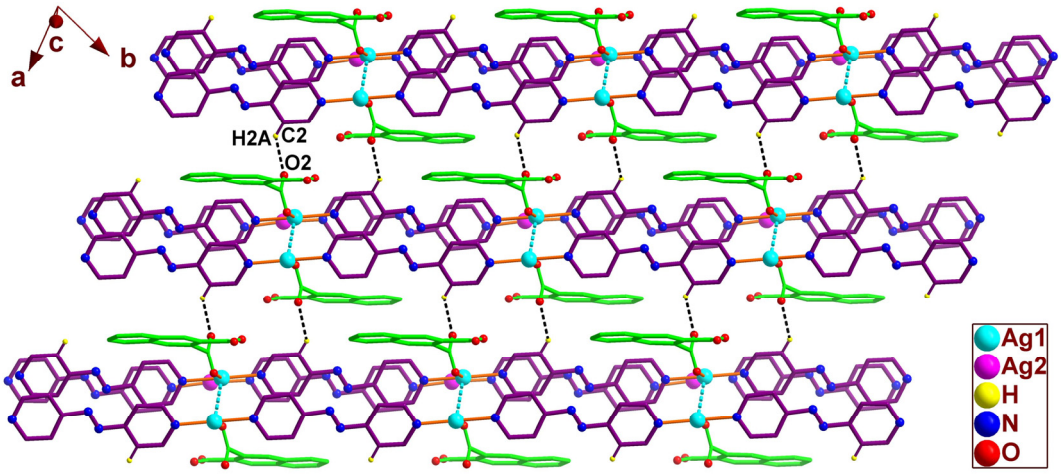


Fig. S10 View of another 2-D layer in **5**, running parallel to the (001) plane, formed by interchain C–H···O (black dashed lines) interactions between **ndc** and abp ligands.

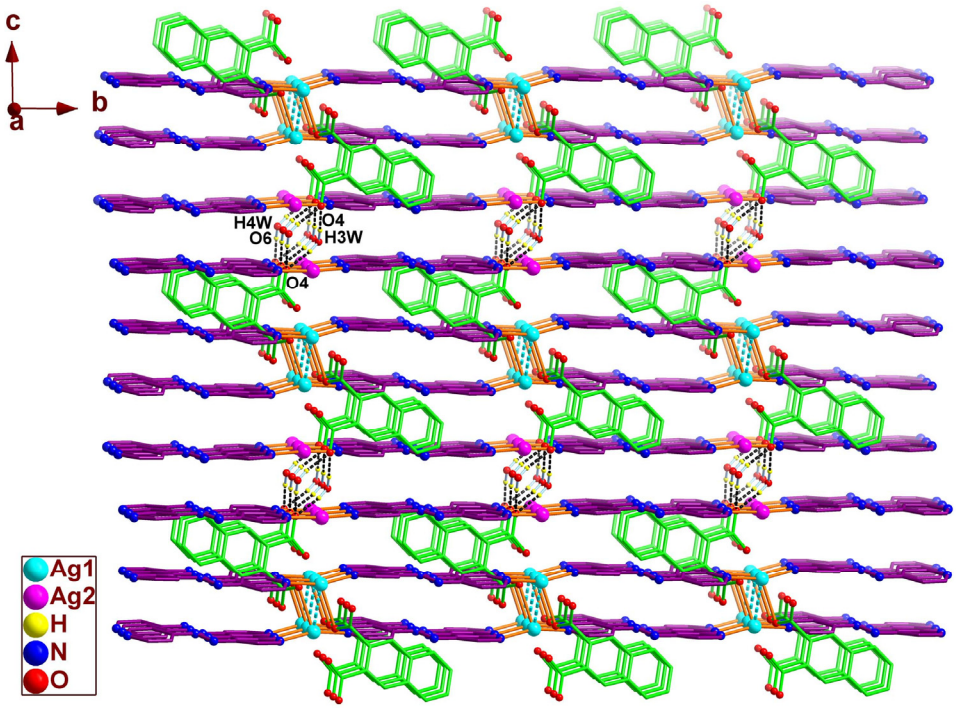


Fig. S11 View of the 3-D supramolecular framework in **5** along the *a* axis.

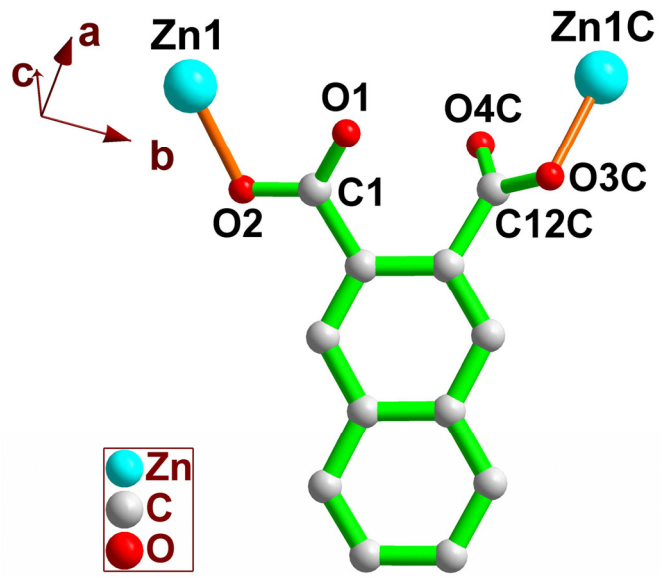


Fig. S12 A portion view of **6** showing the coordination mode of **ndc** (C = $-x + 3/2, y + 1/2, z$).

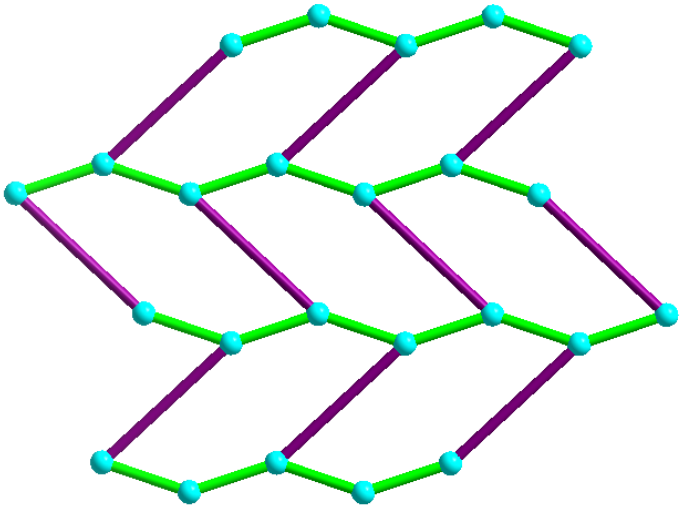


Fig. S13 A schematic representation of the 2-D (6^3) topology in **6** (cyan spheres: Zn^{II}; green rods: **ndc**; purple rods: abp).

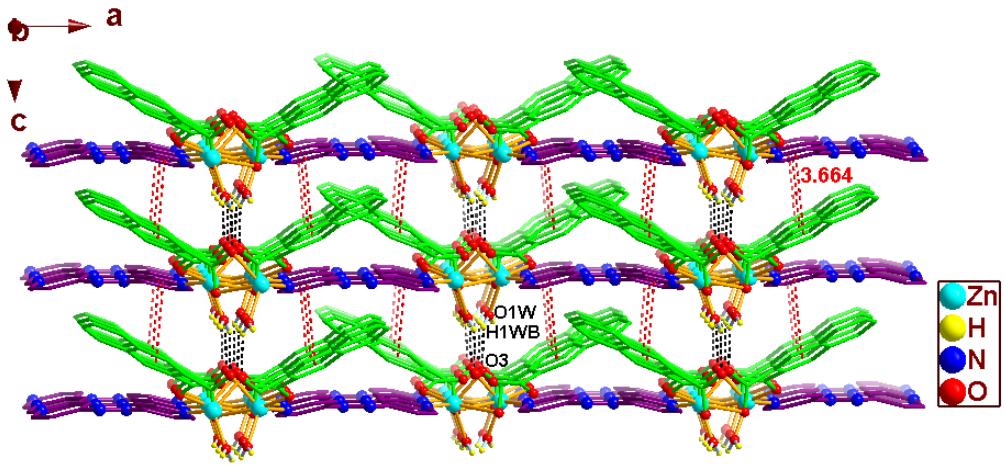
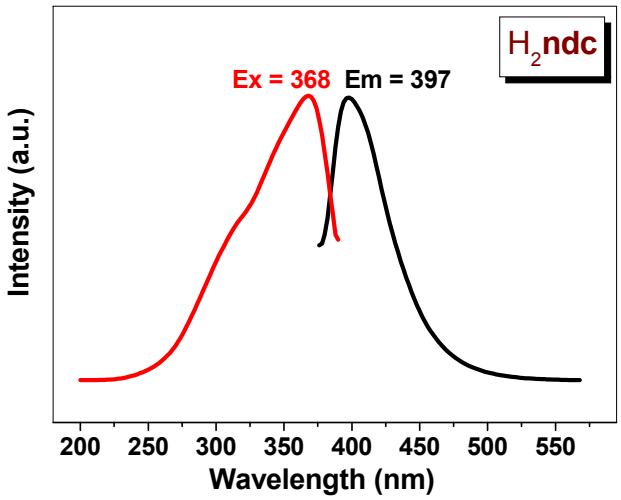
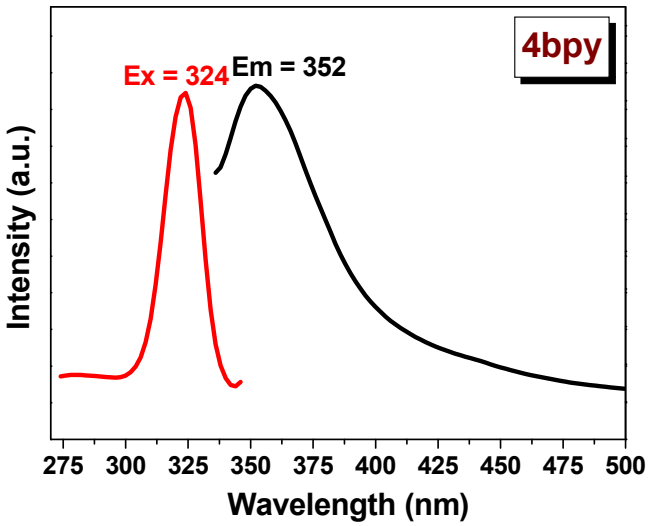


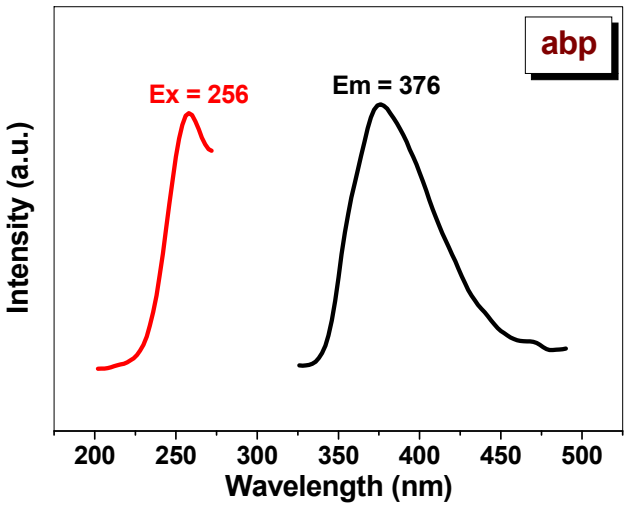
Fig. S14 The 3-D supramolecular net in **6** formed by interlayer O–H···O H-bonding (black dashed lines) and π···π stacking (red dashed lines) interactions.



(a)



(b)



(c)

Fig. S15 Excitation/emission spectra of the free ligands in solid state at room temperature: (a) for H_2**ndc**, (b) for 4bpy, and (c) for abp.

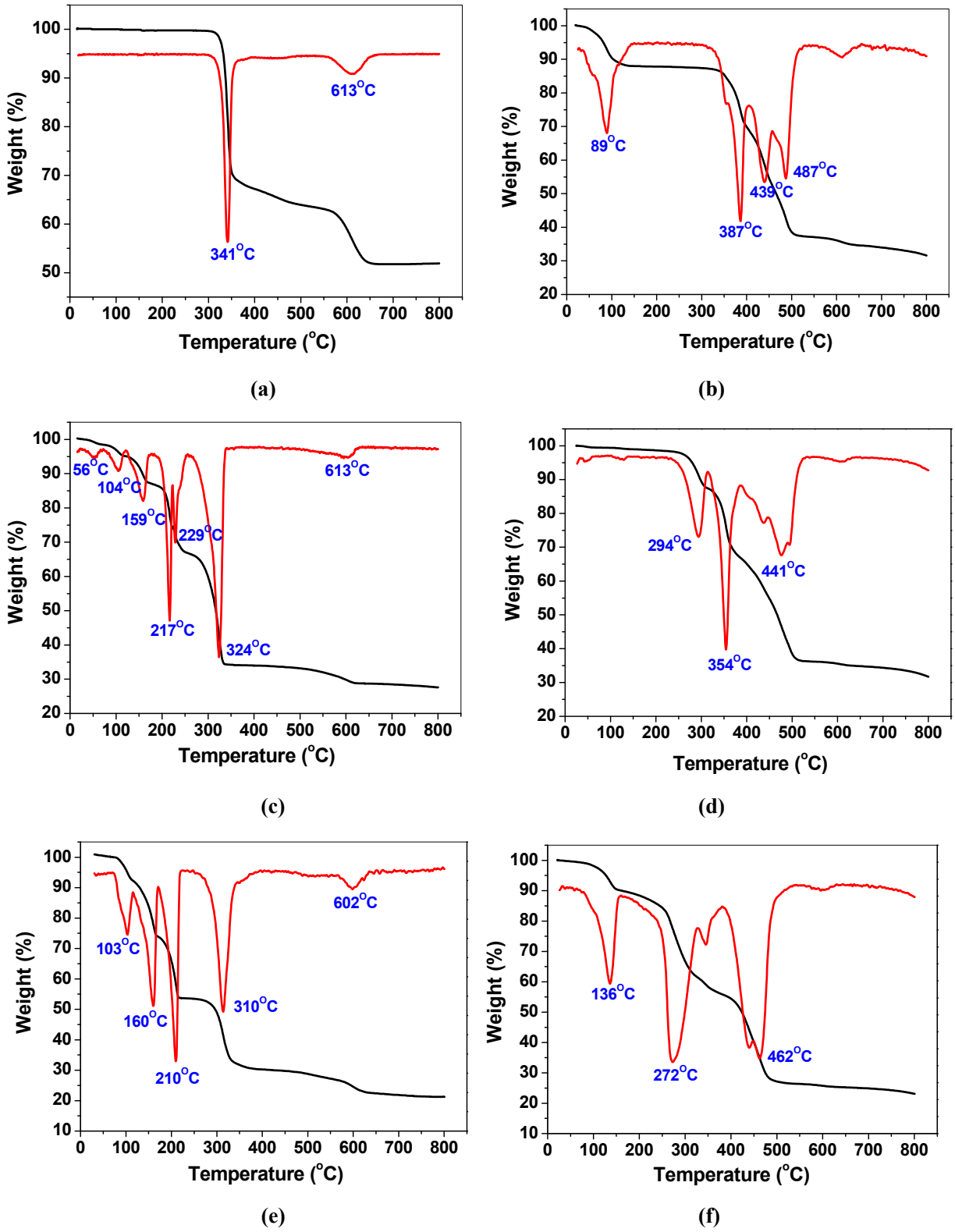


Fig. S16 Thermogravimetric (TG) analysis curves for (a) **1**, (b) **2**, (c) **3**, (d) **4**, (e) **5**, and (f) **6**.

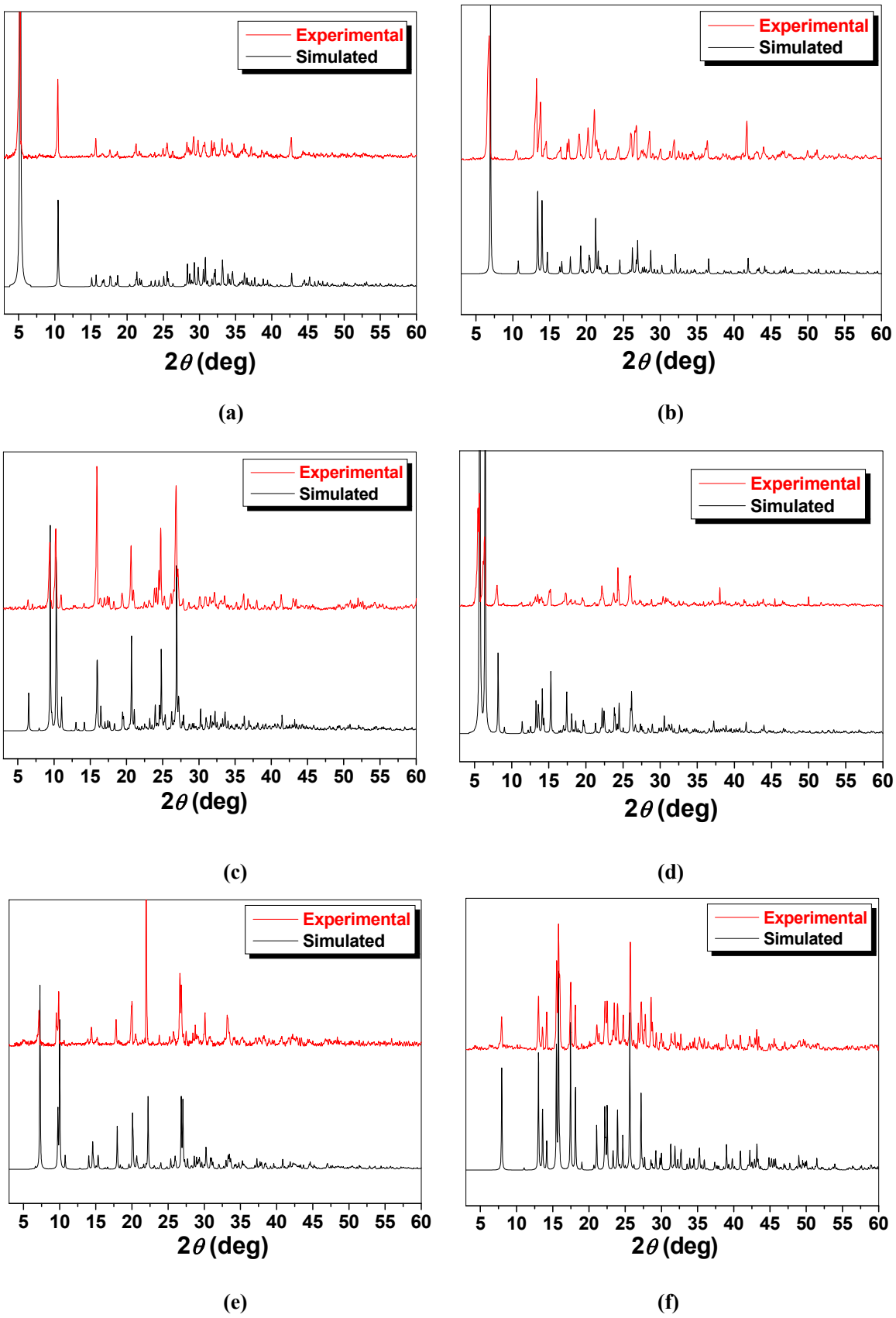


Fig. S17 PXRD patterns for (a) **1**, (b) **2**, (c) **3**, (d) **4**, (e) **5**, and (f) **6**.

Table S1. Selected bond distances (Å) and angles (º) for **1**[a]

Ag1–O4$^{\#1}$	2.222(5)	Ag2–O3$^{\#1}$	2.286(5)
Ag1–O1$^{\#2}$	2.373(6)	Ag2–O2$^{\#4}$	2.317(5)
Ag1–O3	2.392(5)	Ag2–O1	2.368(5)
Ag1–O1$^{\#3}$	2.593(5)	Ag2–O2$^{\#2}$	2.409(6)
Ag1–Ag2	2.9502(9)		
O4$^{\#1}$–Ag1–O1$^{\#2}$	156.74(18)	O3$^{\#1}$–Ag2–O2$^{\#4}$	94.57(19)
O4$^{\#1}$–Ag1–O3	119.6(2)	O3$^{\#1}$–Ag2–O1	149.4(2)
O1$^{\#2}$–Ag1–O3	80.7(2)	O2$^{\#4}$–Ag2–O1	91.69(18)
O4$^{\#1}$–Ag1–O1$^{\#3}$	101.27(18)	O3$^{\#1}$–Ag2–O2$^{\#2}$	95.92(19)
O1$^{\#2}$–Ag1–O1$^{\#3}$	90.55(17)	O2$^{\#4}$–Ag2–O2$^{\#2}$	131.45(11)
O3–Ag1–O1$^{\#3}$	86.59(16)	O1–Ag2–O2$^{\#2}$	102.17(18)
O4$^{\#1}$–Ag1–Ag2	77.27(13)	O3$^{\#1}$–Ag2–Ag1	74.81(13)
O1$^{\#2}$–Ag1–Ag2	82.29(12)	O2$^{\#4}$–Ag2–Ag1	159.03(15)
O3–Ag1–Ag2	121.53(12)	O1–Ag2–Ag1	89.07(12)
O1$^{\#3}$–Ag1–Ag2	148.96(12)	O2$^{\#2}$–Ag2–Ag1	68.55(13)

[a] Symmetry codes for **1**: #1 = x, $-y + 3/2$, $z + 1/2$; #2 = $-x + 1$, $-y + 2$, $-z + 1$; #3 = x, $y - 1$, z; #4 = x, $-y + 5/2$, $z + 1/2$.

Table S2. Selected bond distances (Å) and angles (º) for **2**[a]

Zn1–O2$^{\#1}$	1.959(2)	Zn1–O5	2.0080(19)
Zn1–O1	2.0162(19)	Zn1–O4$^{\#2}$	2.110(2)
Zn1–O3$^{\#2}$	2.230(2)		
O2$^{\#1}$–Zn1–O5	106.54(9)	O2$^{\#1}$–Zn1–O1	95.87(8)
O5–Zn1–O1	94.15(8)	O2$^{\#1}$–Zn1–O4$^{\#2}$	112.53(9)
O5–Zn1–O4$^{\#2}$	92.17(9)	O1–Zn1–O4$^{\#2}$	147.72(8)
O2$^{\#1}$–Zn1–O3$^{\#2}$	153.58(9)	O5–Zn1–O3$^{\#2}$	99.13(9)
O1–Zn1–O3$^{\#2}$	88.28(8)	O4$^{\#2}$–Zn1–O3$^{\#2}$	59.46(7)

[a] Symmetry codes for **2**: #1 = $-x + 1/2, y - 1/2, z$; #2 = $-x, -y, -z + 1$.

Table S3. Selected bond distances (Å) and angles (º) for **3**[a]

Ag1–N1	2.140(4)	Ag2–O3	2.547(3)
Ag1–N2$^{\#1}$	2.147(4)	Ag3–N6	2.196(4)
Ag1–O1	2.582(3)	Ag3–N5$^{\#2}$	2.208(4)
Ag2–N3	2.128(4)	Ag3–O9	2.514(3)
Ag2–N4$^{\#1}$	2.138(4)		
N1–Ag1–N2$^{\#1}$	164.78(15)	N4$^{\#1}$–Ag2–O3	82.22(13)
N1–Ag1–O1	92.48(14)	N6–Ag3–N5$^{\#2}$	154.59(15)
N2$^{\#1}$–Ag1–O1	101.53(14)	N6–Ag3–O9	97.77(13)
N3–Ag2–N4$^{\#1}$	169.34(16)	N5$^{\#2}$–Ag3–O9	99.96(12)
N3–Ag2–O3	107.84(12)		

[a] Symmetry codes for **3**: #1 = x, $-y + 1/2$, $z - 1/2$; #2 = x, $-y + 1/2$, $z + 1/2$.

Table S4. Selected bond distances (Å) and angles (º) for **4**[a]

Zn1–O9	2.039(3)	Zn1–O9$^{\#1}$	2.039(3)
Zn1–O3$^{\#2}$	2.054(4)	Zn1–O3$^{\#3}$	2.054(4)
Zn1–O7$^{\#2}$	2.196(3)	Zn1–O7$^{\#3}$	2.196(3)
Zn2–O4$^{\#3}$	2.027(4)	Zn2–O1	2.049(4)
Zn2–O5$^{\#2}$	2.064(4)	Zn2–O9	2.114(3)
Zn2–O7$^{\#2}$	2.216(4)	Zn2–N1	2.231(4)
Zn3–O9	2.042(3)	Zn3–O2	2.074(4)
Zn3–O8$^{\#3}$	2.117(3)	Zn3–N2	2.129(4)
Zn3–O5	2.180(3)	Zn3–O6	2.369(4)
O9–Zn1–O9$^{\#1}$	180.0	O9–Zn1–O3$^{\#2}$	91.03(14)
O9$^{\#1}$–Zn1–O3$^{\#2}$	8.97(14)	O9–Zn1–O3$^{\#3}$	88.97(14)
O9$^{\#1}$–Zn1–O3$^{\#3}$	91.03(14)	O3$^{\#2}$–Zn1–O3$^{\#3}$	180.00(16)
O9–Zn1–O7$^{\#3}$	81.34(12)	O9$^{\#1}$–Zn1–O7$^{\#3}$	98.66(12)
O3$^{\#2}$–Zn1–O7$^{\#3}$	87.48(14)	O3$^{\#3}$–Zn1–O7$^{\#3}$	92.52(14)
O9–Zn1–O7$^{\#2}$	98.66(12)	O9$^{\#1}$–Zn1–O7$^{\#2}$	81.34(12)
O3$^{\#2}$–Zn1–O7$^{\#2}$	92.52(14)	O3$^{\#3}$–Zn1–O7$^{\#2}$	87.48(14)
O7$^{\#3}$–Zn1–O7$^{\#2}$	180.00(19)	O4$^{\#2}$–Zn2–O1	100.93(16)
O4$^{\#2}$–Zn2–O5$^{\#3}$	163.40(15)	O1–Zn2–O5$^{\#3}$	91.71(15)
O4$^{\#2}$–Zn2–O9	93.06(13)	O1–Zn2–O9	94.55(14)
O5$^{\#3}$–Zn2–O9	96.65(13)	O4$^{\#2}$–Zn2–O7$^{\#3}$	88.07(15)
O1–Zn2–O7$^{\#3}$	169.40(15)	O5$^{\#3}$–Zn2–O7$^{\#3}$	80.58(14)
O9–Zn2–O7$^{\#3}$	79.26(13)	O4$^{\#2}$–Zn2–N1	83.37(15)
O1–Zn2–N1	83.17(16)	O5$^{\#3}$–Zn2–N1	87.54(15)
O9–Zn2–N1	175.30(16)	O7$^{\#3}$–Zn2–N1	103.60(15)
O9–Zn3–O2	98.52(14)	O9–Zn3–O8$^{\#2}$	96.07(14)
O2–Zn3–O8$^{\#2}$	165.16(14)	O9–Zn3–N2	117.62(15)
O2–Zn3–N2	87.41(17)	O8$^{\#2}$–Zn3–N2	88.22(16)
O9–Zn3–O5	93.82(14)	O2–Zn3–O5	92.19(14)
O8$^{\#2}$–Zn3–O5	84.14(13)	N2–Zn3–O5	148.28(16)
O9–Zn3–O6	151.59(13)	O2–Zn3–O6	82.28(15)
O8$^{\#2}$–Zn3–O6	83.60(14)	N2–Zn3–O6	90.79(15)
O5–Zn3–O6	57.82(13)		

[a] Symmetry codes for **4**: #1 = $-x-1, -y+2, -z$; #2 = $-x, -y+2, -z$; #3 = $x-1, y, z$.

Table S5. Selected bond distances (Å) and angles (º) for **5**[a]

Ag1–N1$^{\#1}$	2.177(2)	Ag1–Ag1$^{\#2}$	3.3607(7)
Ag1–N2	2.197(3)	Ag2–N4$^{\#3}$	2.163(2)
Ag1–O1	2.552(3)	Ag2–N3	2.164(2)
N1$^{\#1}$–Ag1–N2	164.79(11)	N2–Ag1–Ag1$^{\#2}$	87.35(8)
N1$^{\#1}$–Ag1–O1	104.27(10)	O1–Ag1–Ag1$^{\#2}$	51.23(6)
N2–Ag1–O1	90.76(9)	N4$^{\#3}$–Ag2–N3	173.13(13)
N1$^{\#1}$–Ag1–Ag1$^{\#2}$	103.80(8)		

[a] Symmetry codes for **5**: #1 = $x - 1, y + 1, z$; #2 = $-x, -y + 2, -z + 1$; #3 = $x + 1, y - 1, z$.

Table S6. Selected bond distances (Å) and angles (º) for **6**

Zn1–O1W	1.957(3)	Zn1–O2	1.979(3)
Zn1–O3	2.038(3)	Zn1–N1	2.064(3)
O1W–Zn1–O2	100.76(13)	O1W–Zn1–O3	123.19(15)
O2–Zn1–O3	114.16(14)	O1W–Zn1–N1	115.40(18)
O2–Zn1–N1	98.73(12)	O3–Zn1–N1	102.33(15)