

Supporting Information for

Synthesis, Structural Characterization and Properties of Ag(I)-Complexes Based on 1,3,4-Oxadiazole Bridging Ligands

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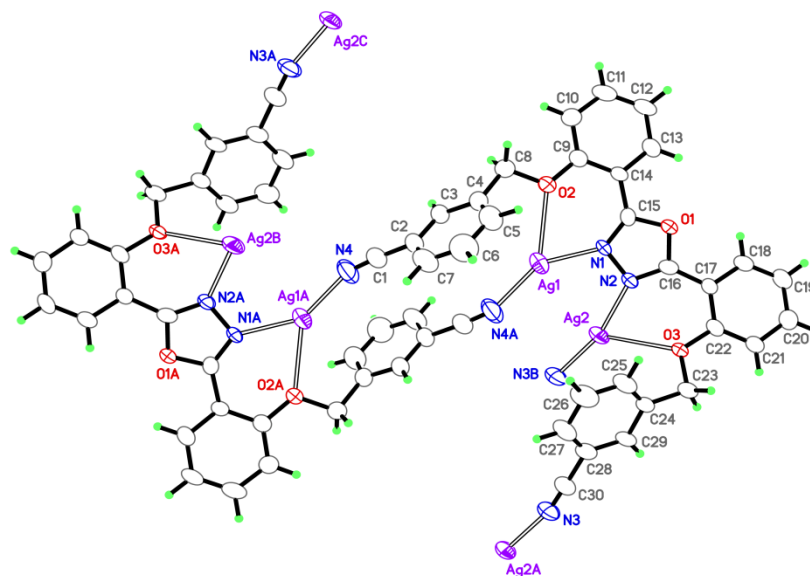


Figure S1. ORTEP figure of **4** (displacement ellipsoids drawn at the 50% probability level. A = -x+1, -y+1, -z; B = -x+1, -y+2, -z; C = x, y-1, z).

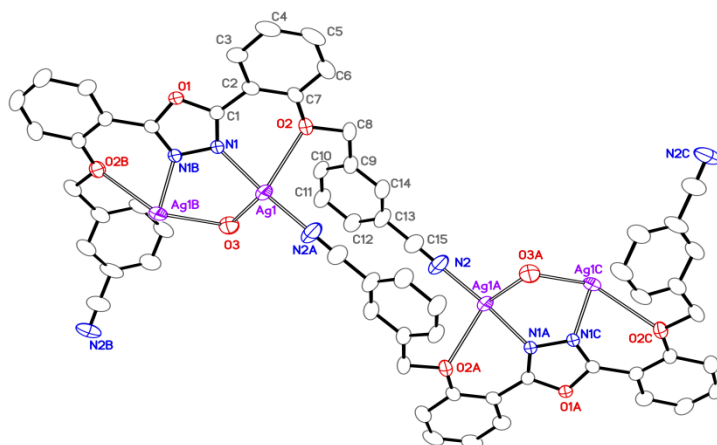


Figure S2. ORTEP figure of **5** (displacement ellipsoids drawn at the 50% probability level. A = -x+2, -y+1, -z+1; B = x, -y+1.5, z; C = -x+2, y-0.5, -z+1).

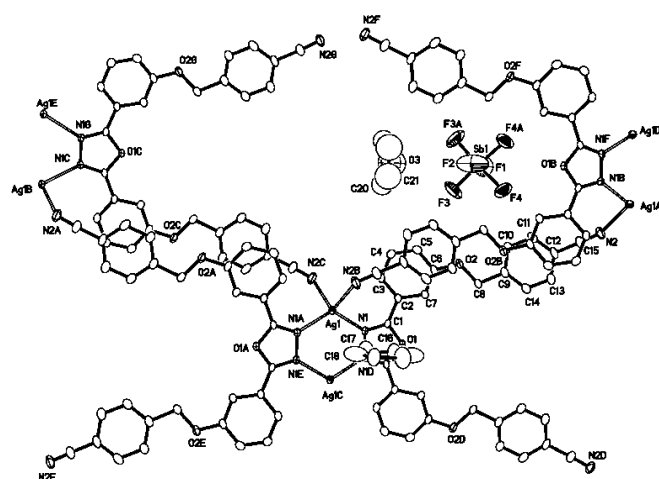


Figure S3. ORTEP figure of **6** (displacement ellipsoids drawn at the 50% probability level. A = -x+1, y, -z+1; B = -x+0.5, -y+0.5, -z+2; C = x+0.5, -y+0.5, z-1; D = x, -y+1, z; E = -x+1, -y+1, -z+1; F = -x+0.5, y-0.5, -z+2).

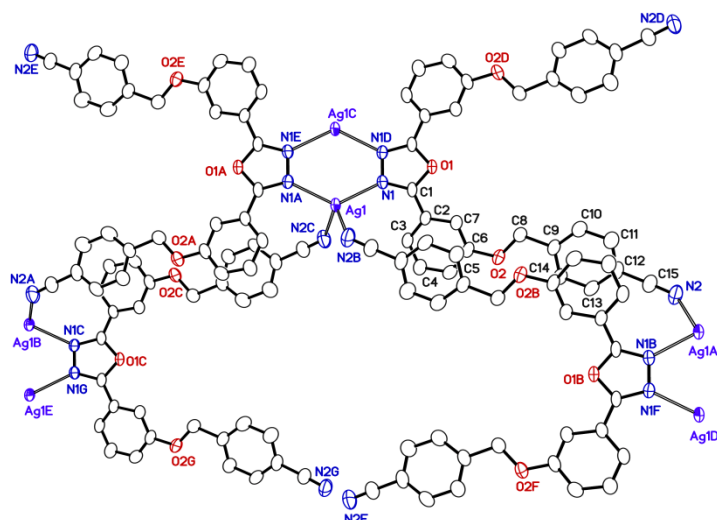


Figure S4. ORTEP figure of **7** (displacement ellipsoids drawn at the 50% probability level. A= $-x+1, y, -z$; B = $-x+0.5, -y+0.5, -z+1$; C = $x+0.5, -y+0.5, z-1$; D = $x, -y, z$; E = $-x+1, -y, -z$; F = $-x+0.5, y+0.5, -z+1$; G = $x+0.5, y+0.5, z-1$).

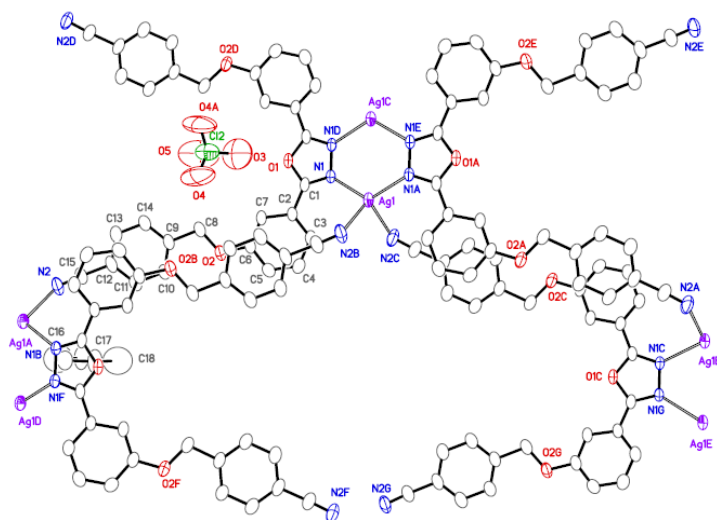


Figure S5. ORTEP figure of **8** (displacement ellipsoids drawn at the 50% probability level. A = $-x, y, z$; B = $-x+0.5, -y+0.5, -z+1$; C = $x-0.5, -y+0.5, z-1$; D = $x, -y, z$; E = $-x, -y, -z$; F = $-x+0.5, y+0.5, -z+1$).

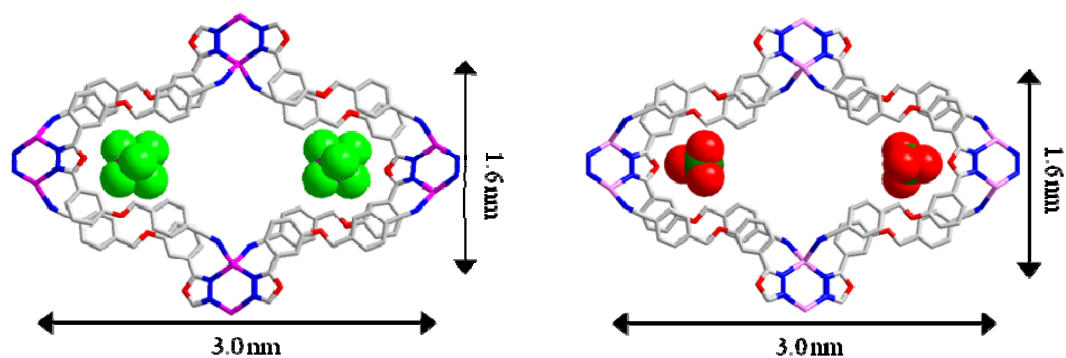


Figure S6. Ag(I)-L3 macrocyclic units of **7** (left) and **8** (right).

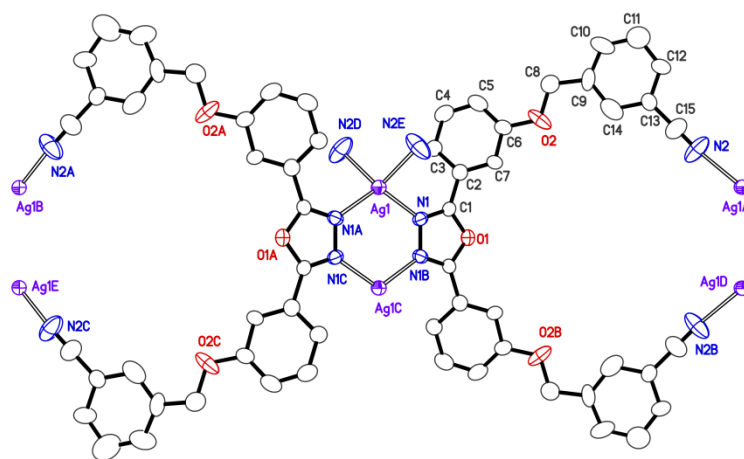


Figure S7. ORTEP figure of **9** (displacement ellipsoids drawn at the 50% probability level. A = -x+1, y, -z; B = x, -y+1, z; C = -x+1, -y+1, -z; D = x, y, z-1; E = -x+1, y, -z+1).

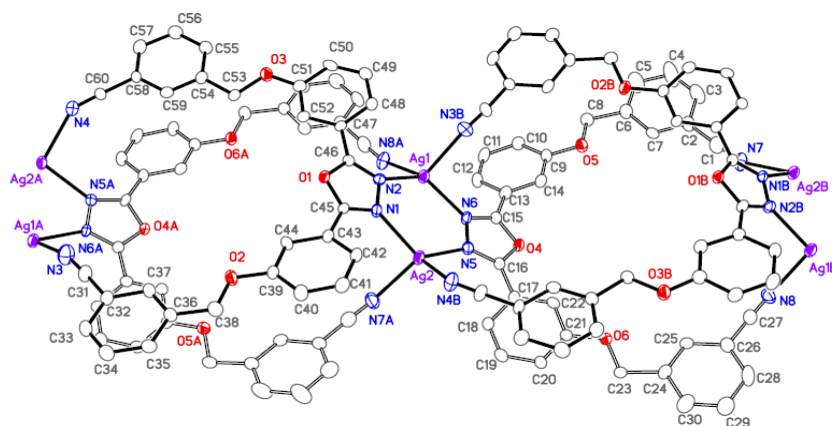


Figure S8. ORTEP figure of **10** (displacement ellipsoids drawn at the 50% probability level. A = x, -y, z+0.5; B = x,

-y, z-0.5).

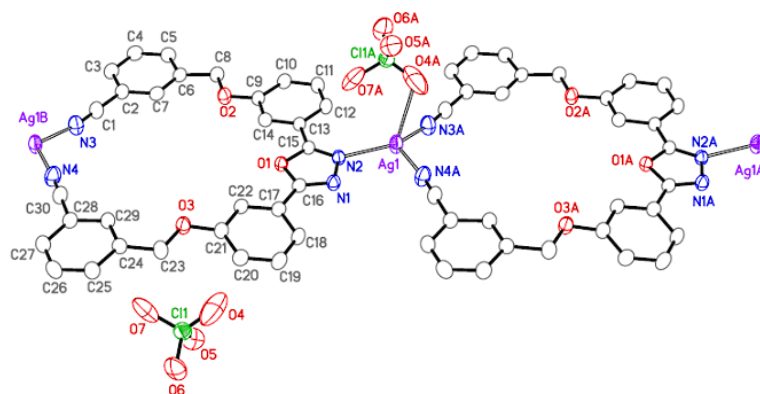


Figure S9. ORTEP figure of **11** (displacement ellipsoids drawn at the 50% probability level. A = x, y+1, z; B = x, y-1, z).

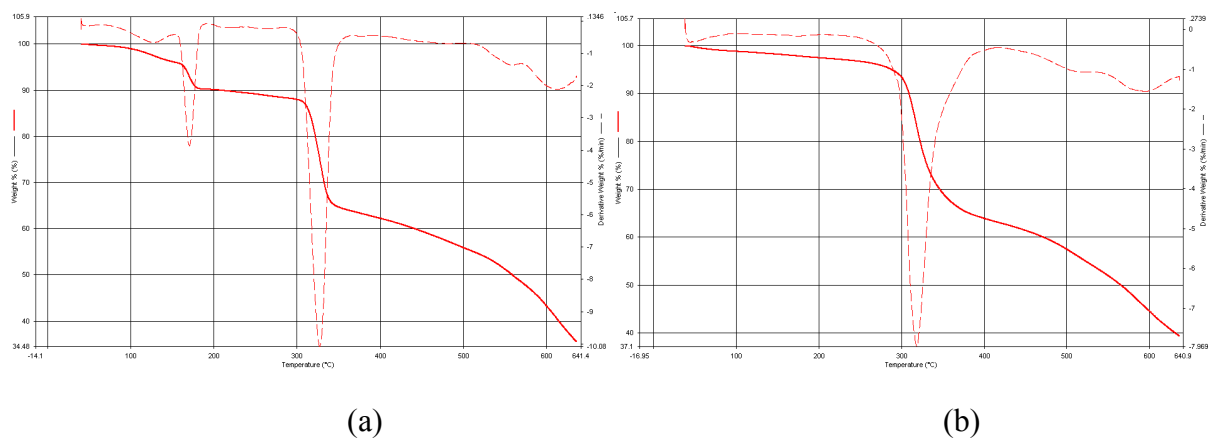


Figure S10. TGA traces of as-synthesized **6** (a) and desolvated **6a** (b). Benzene and THF guest molecules can be removed at 100~180°C (a), and the desolvated sample of **6a** was obtained by heating crystals of **6** at 110°C for about 12 hours (b).

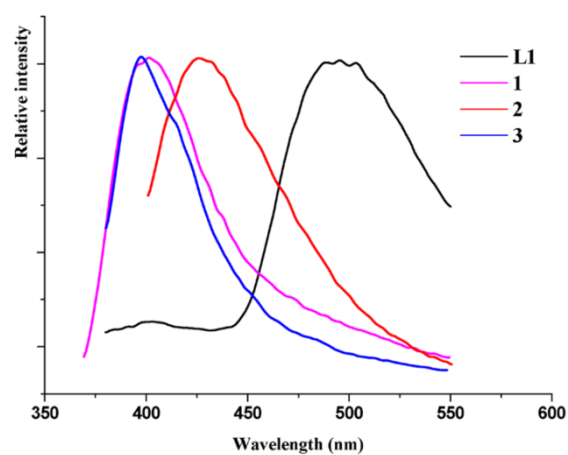


Figure S11. Photoinduced emission spectra of **L1** and **1-3** in the solid state.

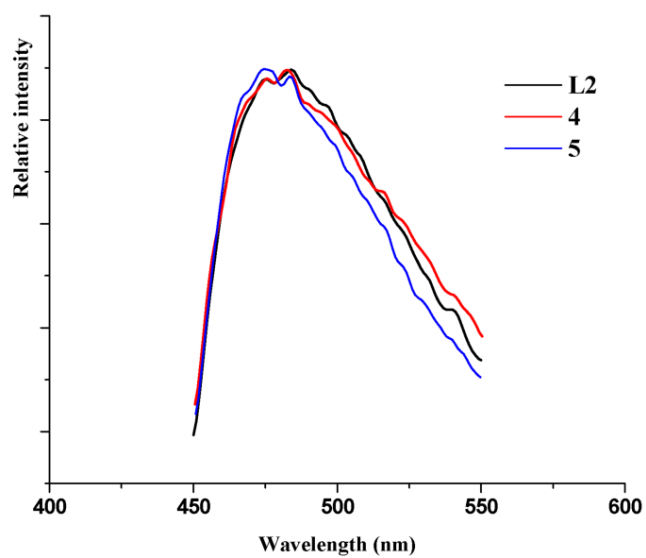


Figure S12. Photoinduced emission spectra of **L2** and **4-5** in the solid state.

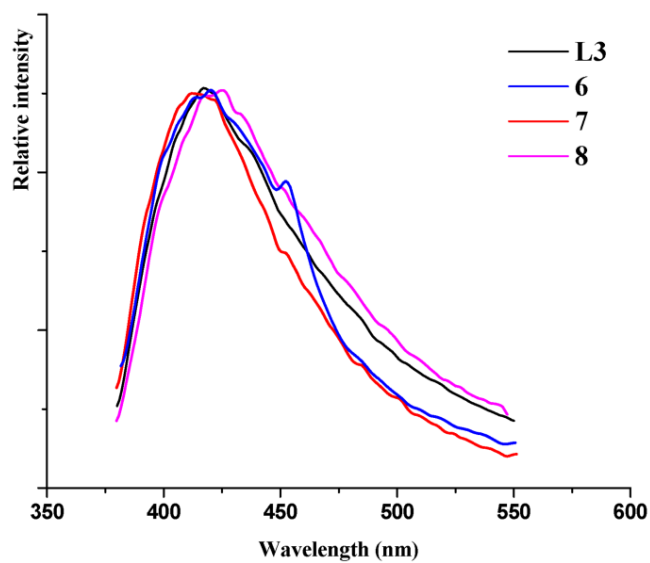


Figure S13. Photoinduced emission spectra of **L3** and **6-8** in the solid state.

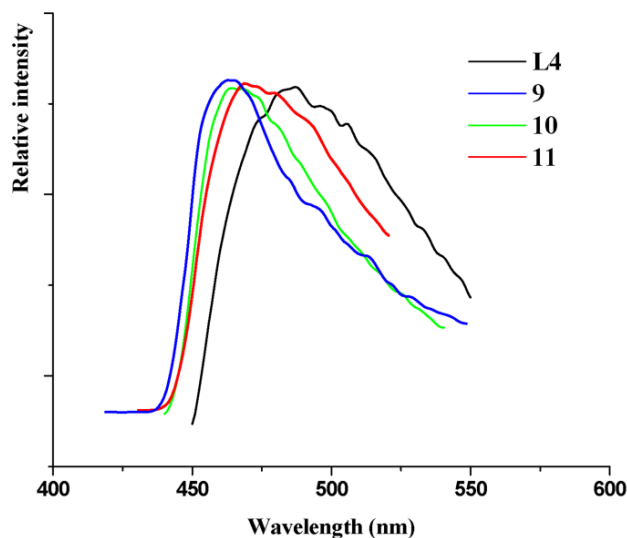


Figure S14. Photoinduced emission spectra of **L4** and **9-11** in the solid state.

Table S1. Interatomic Distances (Å) and Bond Angles (°) with esds () for **1**.

Ag(1)-N(1)	2.247(4)	Ag(1)-N(1)#1	2.247(4)
Ag(1)-O(2)	2.608(6)	Ag(1)-O(2)#1	2.608(6)
N(1)-Ag(1)-N(1)#1	122.7(2)	N(1)-Ag(1)-O(2)	68.93(2)
O(2)-Ag(1)-O(2)#1	113.03(4)	O(2)-Ag(1)-N(1)#1	152.70(7)

Symmetry transformations used to generate equivalent atoms:

- | | |
|--------------------|-------------------|
| #1 -x+3/2,-y+1/2,z | #2 -x+1,-y+1,-z+2 |
| #3 -x+1/2,-y+1/2,z | #4 -x+1/2,y,-z+2 |
| #5 x,-y+1/2,-z+1 | #6 -x+3/2,y,-z+2 |
| #7 x,-y+1/2,-z+2 | #8 -x+1/2,y,-z+1 |

Table S2. Interatomic Distances (Å) and Bond Angles (°) with esds () for **2**.

Ag(1)-N(1)#1	2.210(3)	Ag(1)-N(3)#2	2.283(4)
Ag(1)-N(2)	2.337(4)	Ag(1)-O(1)	2.793(3)
Ag(1)-O(2)#1	2.696(3)		
N(1)#1-Ag(1)-N(3)#2	133.42(14)	N(3)#2-Ag(1)-N(2)	92.18(14)
N(1)#1-Ag(1)-N(2)	119.96(12)		

Symmetry transformations used to generate equivalent atoms:

- | | | |
|-----------------|------------|------------|
| #1 -x+1,-y,-z+1 | #2 x-1,y,z | #3 x+1,y,z |
|-----------------|------------|------------|

Table S3. Interatomic Distances (Å) and Bond Angles (°) with esds () for **3**.

Ag(1)-N(2)	2.277(3)	Ag(1)-N(3)#1	2.285(3)
Ag(1)-N(1)#2	2.322(3)	Ag(1)-O(4)	2.566(3)
N(1)-Ag(1)#2	2.322(3)	N(3)-Ag(1)#3	2.285(3)
N(2)-Ag(1)-N(3)#1	127.65(11)	N(2)-Ag(1)-N(1)#2	113.58(9)
N(3)#1-Ag(1)-N(1)#2	117.84(10)	N(2)-Ag(1)-O(4)	100.64(9)
N(3)#1-Ag(1)-O(4)	94.27(9)	N(1)#2-Ag(1)-O(4)	83.47(9)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 -x,-y+2,-z #3 x,y,z+1 #4 -x+2,-y+1,-z+1

Table S4. Interatomic Distances (Å) and Bond Angles (°) with esds () for **4**.

Ag(1)-N(4)#1	2.161(7)	Ag(1)-N(1)	2.197(5)
Ag(2)-N(3)#2	2.115(6)	Ag(2)-N(2)	2.174(5)
N(3)-Ag(2)#2	2.115(6)	N(4)-Ag(1)#1	2.161(7)
Ag(1)-O(2)	2.619(5)	Ag(2)-O(3)	2.652(6)
N(4)#1-Ag(1)-N(1)	141.1(3)	N(3)#2-Ag(2)-N(2)	163.9(2)
N(1)-Ag(1)-O(2)#1	71.52(17)	O(2)-Ag(1)-N(1)#1	142.48(21)
N(2)-Ag(2)-O(3)	70.20 (16)	N(3)-Ag(2)-O(3)	125.82(21)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x+1,-y+2,-z

Table S5. Interatomic Distances (Å) and Bond Angles (°) with esds () for **5**.

Ag(1)-N(2)#1	2.152(4)	Ag(1)-N(1)	2.226(3)
Ag(1)-O(2)	2.774(4)	Ag(1)-O(3)	2.475(4)
Ag(1)-O(4)#3	2.654(4)		
N(2)#1-Ag(1)-N(1)	169.06(17)	N(1)-Ag(1)-O(2)	69.11(13)
N(1)-Ag(1)-O(3)	90.33(14)	N(1)-Ag(1)-O(4)#3	81.45(14)
N(2)#1-Ag(1)-O(2)	107.10(16)	N(2)#1-Ag(1)-O(3)	99.81(19)
N(2)#1-Ag(1)-O(4)#3	90.29 (17)	O(2)-Ag(1)-O(3)	127.27(7)
O(3)-Ag(1)-O(4)#3	116.49(13)	O(2)-Ag(1)-O(4)#3	107.95(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1 #2 x,-y+3/2,z #3 x+1,y,z

Table S6. Interatomic Distances (Å) and Bond Angles (°) with esds () for **6**.

Ag(1)-N(1)#1	2.275(4)	Ag(1)-N(1)	2.275(4)
Ag(1)-N(2)#2	2.392(6)	Ag(1)-N(2)#3	2.392(6)
N(2)-Ag(1)#3	2.392(6)		
N(1)#1-Ag(1)-N(1)	122.5(2)	N(1)#1-Ag(1)-N(2)#2	103.52(18)
N(1)-Ag(1)-N(2)#2	113.04(18)	N(1)#1-Ag(1)-N(2)#3	113.04(18)
N(1)-Ag(1)-N(2)#3	103.52(18)	N(2)#2-Ag(1)-N(2)#3	98.9(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1 #2 x+1/2,-y+1/2,z-1

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

#5 -x+1,-y+1,-z+2 #6 x,-y,z

Table S7. Interatomic Distances (Å) and Bond Angles (°) with esds () for **7**.

Ag(1)-N(1)#1	2.280(3)	Ag(1)-N(1)	2.280(3)
Ag(1)-N(2)#2	2.397(5)	Ag(1)-N(2)#3	2.397(5)
N(2)-Ag(1)#2	2.397(5)		
N(1)#1-Ag(1)-N(1)	122.93(19)	N(1)#1-Ag(1)-N(2)#2	112.52(14)
N(1)-Ag(1)-N(2)#2	104.05(14)	N(1)#1-Ag(1)-N(2)#3	104.05(14)
N(1)-Ag(1)-N(2)#3	112.52(14)	N(2)#2-Ag(1)-N(2)#3	98.2(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z #2 -x+1/2,-y+1/2,-z+1

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

#5 x,-y,z #6 x,-y+1,z

Table S8. Interatomic Distances (Å) and Bond Angles (°) with esds () for **8**.

Ag(1)-N(1)#1	2.306(4)	Ag(1)-N(1)	2.306(4)
Ag(1)-N(2)#2	2.427(5)	Ag(1)-N(2)#3	2.427(5)
N(2)-Ag(1)#2	2.427(5)		
N(1)#1-Ag(1)-N(1)	124.09(17)	N(1)#1-Ag(1)-N(2)#2	111.81(14)
N(1)-Ag(1)-N(2)#2	103.80(13)	N(1)#1-Ag(1)-N(2)#3	103.80(13)
N(1)-Ag(1)-N(2)#3	111.81(14)	N(2)#2-Ag(1)-N(2)#3	98.8(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z #2 -x+1/2,-y+1/2,-z+1

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

Table S9. Interatomic Distances (Å) and Bond Angles (°) with esds () for **9**.

Ag(1)-N(1)#1	2.266(7)	Ag(1)-N(1)	2.266(7)
Ag(1)-N(2)#2	2.312(12)	Ag(1)-N(2)#3	2.312(12)
N(2)-Ag(1)#5	2.312(12)		
N(1)#1-Ag(1)-N(1)	119.9(4)	N(1)#1-Ag(1)-N(2)#2	96.2(4)
N(1)-Ag(1)-N(2)#2	120.3(4)	N(1)#1-Ag(1)-N(2)#3	120.3(4)
N(1)-Ag(1)-N(2)#3	96.2(4)	N(2)#2-Ag(1)-N(2)#3	104.4(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z #2 x,y,z-1 #3 -x+1,y,-z+1

#4 x,-y+1,z #5 x,y,z+1

Table S10. Interatomic Distances (Å) and Bond Angles (°) with esds () for **10**.

Ag(1)-N(6)	2.228(6)	Ag(1)-N(8)#1	2.251(7)
Ag(1)-N(2)	2.275(7)	Ag(1)-N(3)#2	2.349(7)
Ag(2)-N(5)	2.253(6)	Ag(2)-N(7)#1	2.277(7)
Ag(2)-N(1)	2.319(6)	Ag(2)-N(4)#2	2.358(7)
N(3)-Ag(1)#1	2.349(7)	N(4)-Ag(2)#1	2.358(7)
N(5)-N(6)	1.401(9)	N(7)-Ag(2)#2	2.277(7)
N(8)-Ag(1)#2	2.251(7)		
N(6)-Ag(1)-N(8)#1	125.2(2)	N(6)-Ag(1)-N(2)	119.88(17)
N(8)#1-Ag(1)-N(2)	95.7(2)	N(6)-Ag(1)-N(3)#2	97.0(3)
N(8)#1-Ag(1)-N(3)#2	104.4(3)	N(2)-Ag(1)-N(3)#2	114.6(3)
N(5)-Ag(2)-N(7)#1	127.7(2)	N(5)-Ag(2)-N(1)	120.06(17)
N(7)#1-Ag(2)-N(1)	95.7(2)	N(5)-Ag(2)-N(4)#2	101.9(2)
N(7)#1-Ag(2)-N(4)#2	97.3(3)	N(1)-Ag(2)-N(4)#2	112.3(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y,z-1/2 #2 x,-y,z+1/2

Table S11. Interatomic Distances (Å) and Bond Angles (°) with esds () for **11**.

Ag(1)-N(3)#1	2.185(5)	Ag(1)-N(2)	2.248(3)
Ag(1)-N(4)#1	2.294(5)	N(3)-Ag(1)#2	2.185(5)
N(4)-Ag(1)#2	2.294(5)	Ag(1)-O(4)#1	2.782(8)
N(3)#1-Ag(1)-N(2)	138.33(15)	N(3)#1-Ag(1)-N(4)#1	119.10(18)
N(2)-Ag(1)-N(4)#1	99.82(15)		

Symmetry transformations used to generate equivalent atoms:

#1 x,-y,z-1/2 #2 x,-y,z+1/2

Refinement details:

- (1) **Compound 1:** All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms. In the title molecule, half a solvent benzene molecule was disordered and total 11 geometric restraints were used in modeling the solvent molecules.
- (2) **Compound 2:** All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms. In the title molecule, some diffuse species are assumed to be several disordered solvent molecules. SQUEEZE / PLATON was used to account for these species. The contribution of these disordered species was then removed from the structure factor calculations.
- (3) **Compound 3:** All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms. In the title molecule, there were some disordered solvent molecules besides benzene solvent molecule. SQUEEZE / PLATON was used to account for these. The contribution of these disordered solvent was then removed from the structure factor calculations.
- (4) **Compound 4:** All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93, 0.97 Å for aromatic and methylene H, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms.
- (5) **Compound 5:** All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to carbon were placed in idealized positions and included as riding atoms, with C-H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms. The water hydrogen atoms were also located and were refined with a

common isotropic displacement parameter with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. The triflate ion was also severely disordered and 18 restraints were used to model it. A large void space is present between the frameworks, which contains many significant electron density peaks. The species in this region were too severely disordered to be modeled. SQUEEZE / PLATON was used to account for these species. The program calculated a solvent accessible void volume of $148.9 \text{ \AA}^3$ corresponding to $41 \text{ e}^-/\text{cell}$. The contribution of these disordered species was then removed from the structure factor calculations..

- (6) **Compound 6:** All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93, 0.97 Å for aromatic and methylene H, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms. There were one THF and half of a benzene molecular were located in the framework. Total 16 geometric restraints were used in modeling these solvent molecules.
- (7) **Compound 7:** All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93, 0.97 Å for aromatic and methylene H, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms. Half of a benzene molecule was located in the framework. Total 8 geometric restraints were used in modeling these benzene rings. There were other disordered solvent molecules in the framework. SQUEEZE / PLATON was used to account for these molecules. The program calculated a solvent accessible void volume of $1074.5 \text{ \AA}^3$ corresponding to $67 \text{ e}^-/\text{cell}$. The contribution of these disordered species was then removed from the structure factor calculations.
- (8) **Compound 8:** The date was treated newly. It is not a twin. The space group is monoclinic, $C2/m$. And $_cell_angle_beta$ is 90.02(2). All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to carbon were placed in idealized positions and included as riding atoms, with C—H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms . 12 geometric restraints were used in modeling the Solvent Benzene molecule. There were other disordered solvent molecules in the framework. SQUEEZE / PLATON was used to account for

these species. The program calculated a solvent accessible void volume of 1140.8 Å³ corresponding to 47 e⁻/cell. The contribution of these disordered species was then removed from the structure factor calculations.

- (9) Compound **9**: All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93, 0.97 Å for aromatic and methylene H, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms. Total 21 geometric restraints were used in modeling the Benzene ring.
- (10) Compound **10**: All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93, 0.97 Å for aromatic and methylene H, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms. In the title molecule, one THF was located in the framework. Total 36 geometric restraints were used in modeling the solvent molecules.
- (11) Compound **11**: All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to refined atoms were placed in geometrically idealized positions and refined using a riding model, with C-H = 0.93, 0.97 Å for aromatic and methylene H, respectively, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all H atoms. In the title molecule, one CH₂Cl₂ and one water molecules were disordered with refined site occupation factors of 0.5 / 0.5. The C-Cl bond lengths were restrained from 1.613 to 1.674 Å. Total two geometric restraints were used in modeling the disorder solvent molecules.