

Supplementary Material (ESI) for Dalton Transactions
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Three 3D Silver-bis(triazole) Metal-organic Frameworks

Stabilized by High-connected Wells-Dawson

Polyoxometallate

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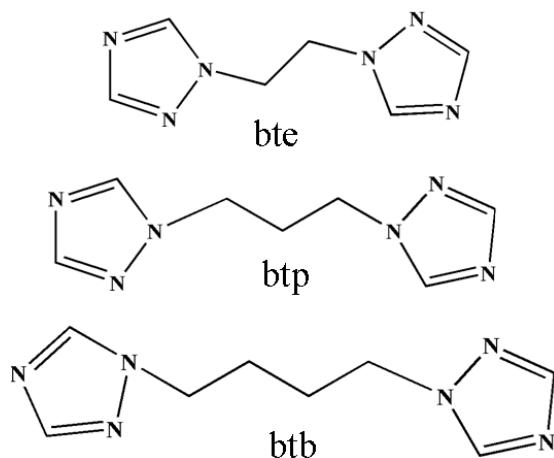


Chart S1. The organic ligands 1,2-bis(1,2,4-triazol-1-yl)ethane (bte), 1,3-bis(1,2,4-triazol-1-yl)propane (btp) and 1,4-bis(1,2,4-triazol-1-yl)butane (btb) used in compounds **1–3**.

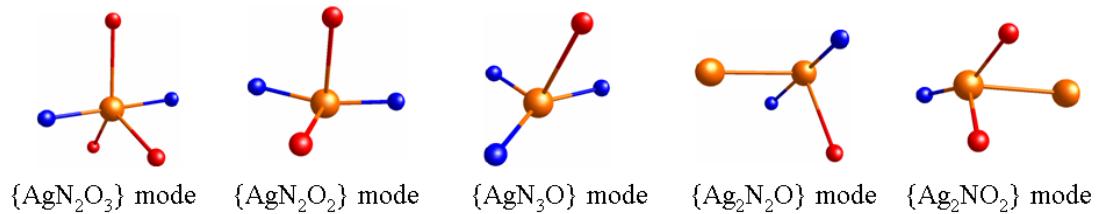


Figure S1. Five coordination modes of Ag^I ions in compound **1**.

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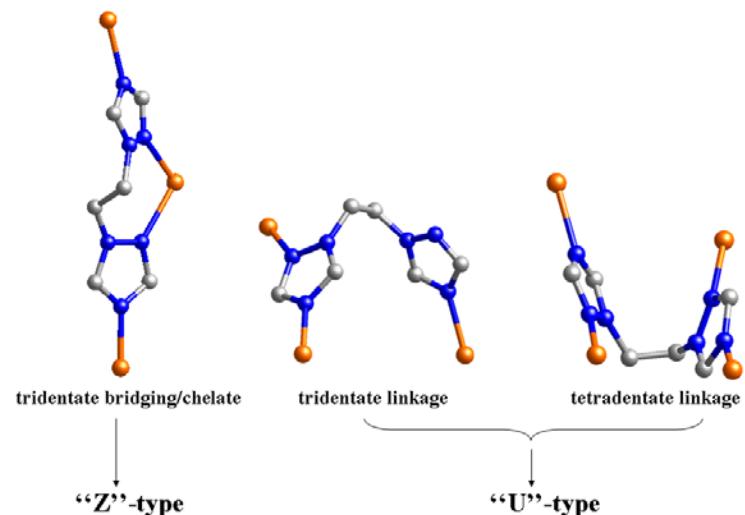


Figure S2. The conformation and coordination modes of bte in compound **1**.

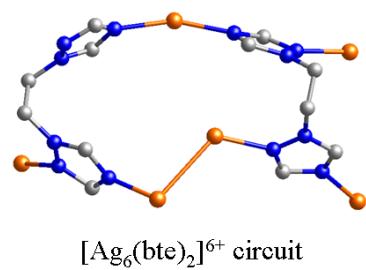


Figure S3. The $[Ag_6(bte)_2]^{6+}$ circuit in compound **1**.

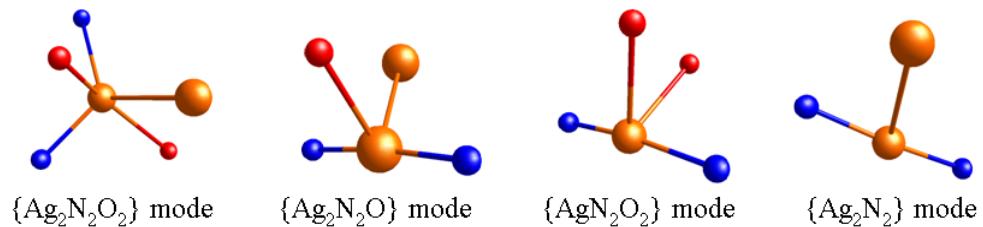


Figure S4. Four coordination modes of Ag^I ions in compound **2**.

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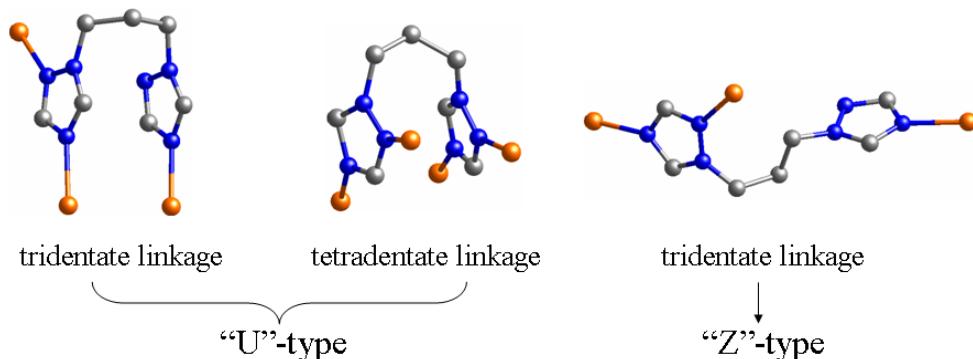


Figure S5. The conformations and coordination modes of btp in compound **2**.

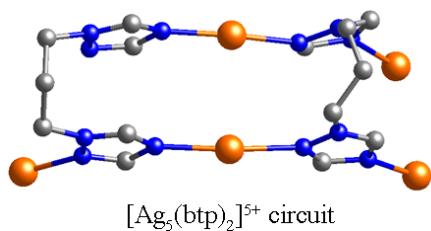


Figure S6. The $[\text{Ag}_5(\text{btp})_2]^{5+}$ circuit in compound **2**.

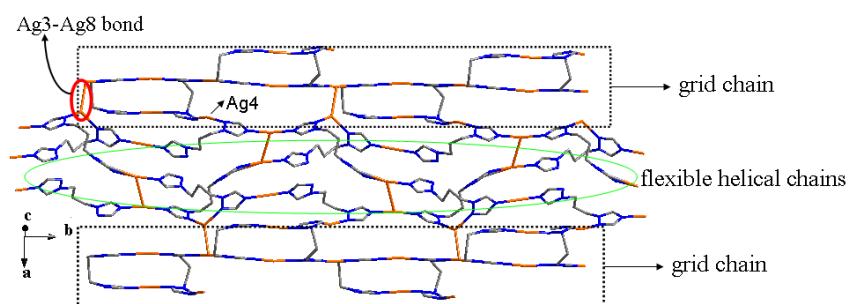


Figure S7. Detailed instructions for the 2D Ag/btp layer in **2**.

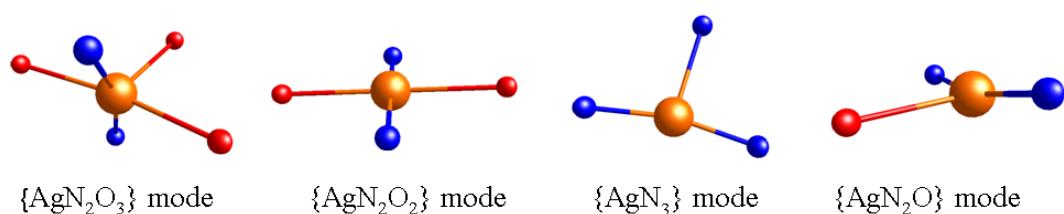


Figure S8. Four coordination modes of Ag^{I} ions in compound **3**.

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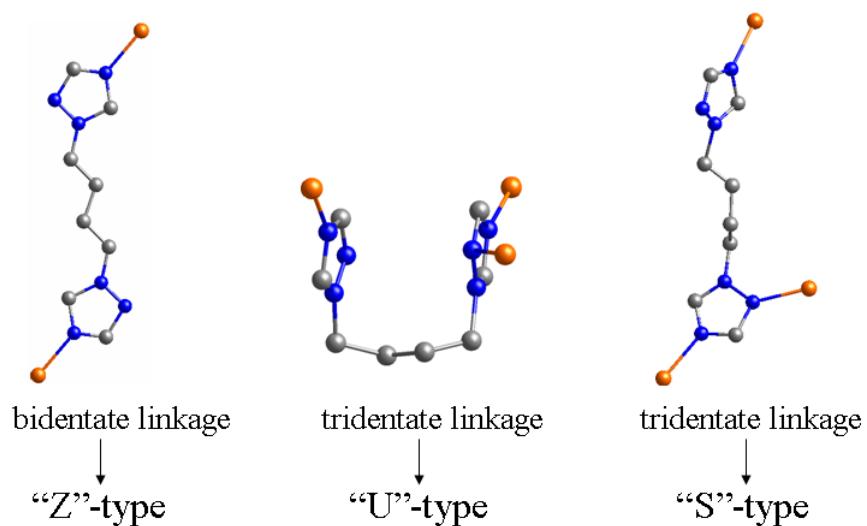


Figure S9. The conformations and coordination modes of btb in compound 3.

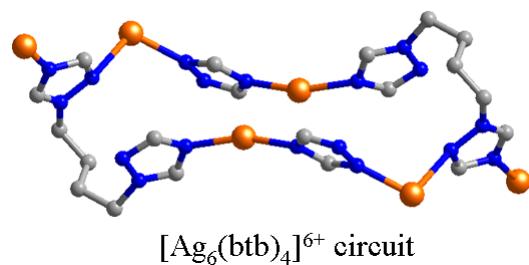
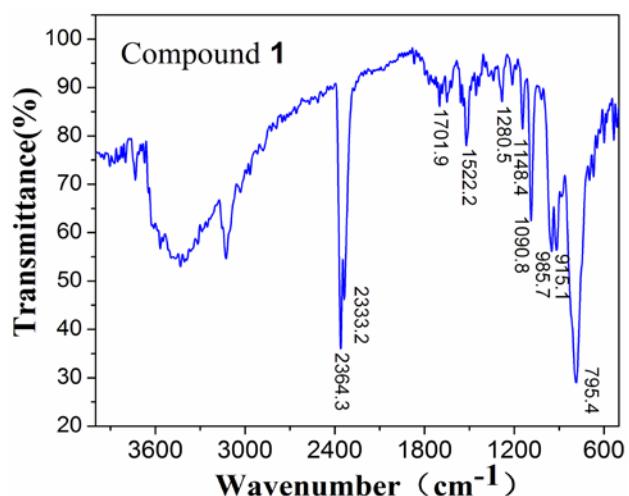


Figure S10. The $[Ag_6(btb)_4]^{6+}$ circuit in compound 3.



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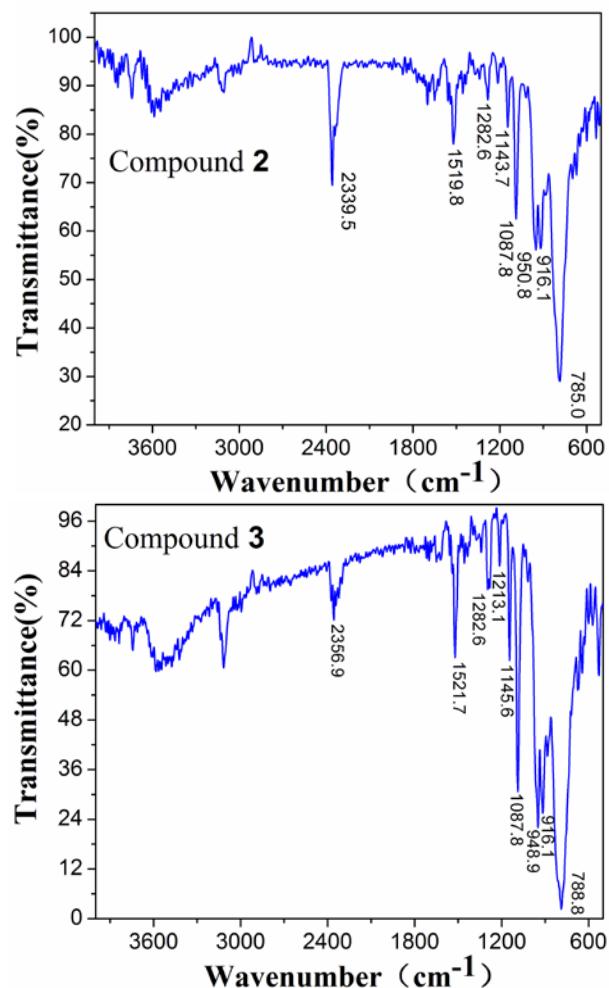
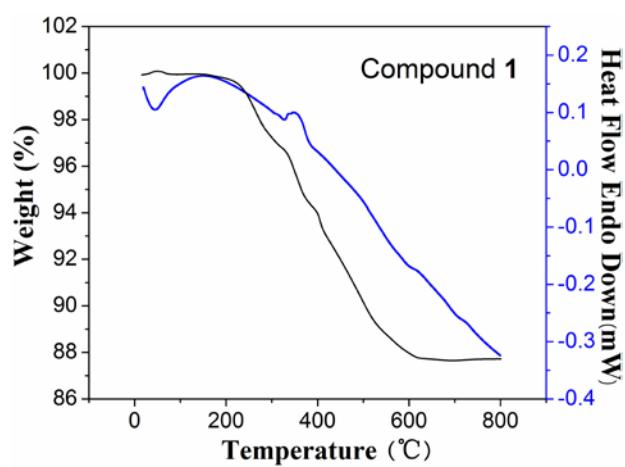


Figure S11. The IR spectra of compounds **1–3**.



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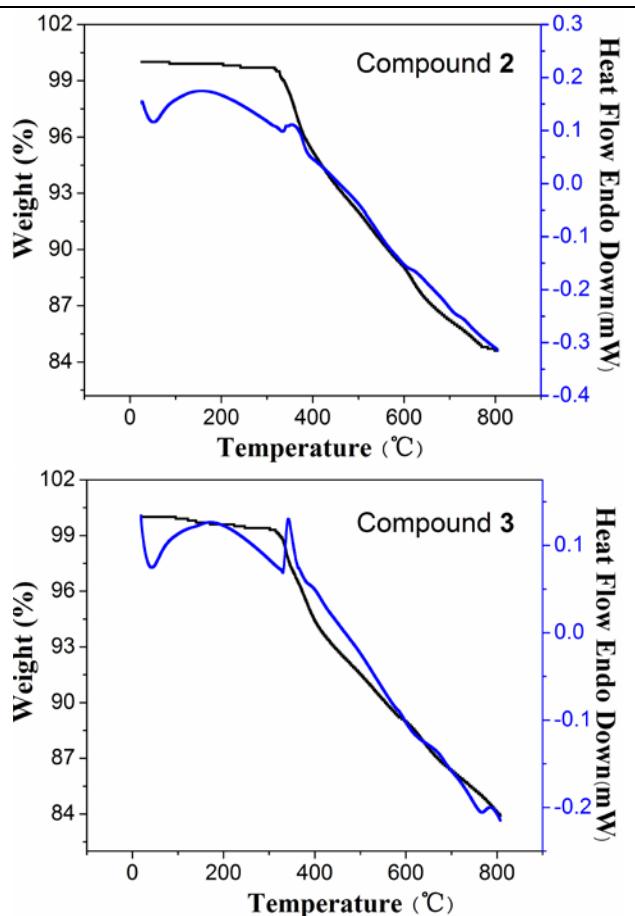


Figure S12. The TG (black) and DTA (blue) curves of compounds **1–3**.

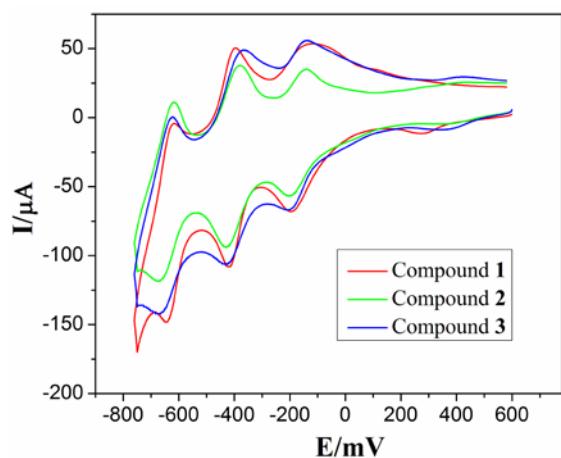


Figure S13. The cyclic voltammograms of the **1–**, **2–** and **3–**CPEs in 0.1M H₂SO₄ + 0.5M Na₂SO₄ aqueous solution at scan rate of 160 mV·s⁻¹.

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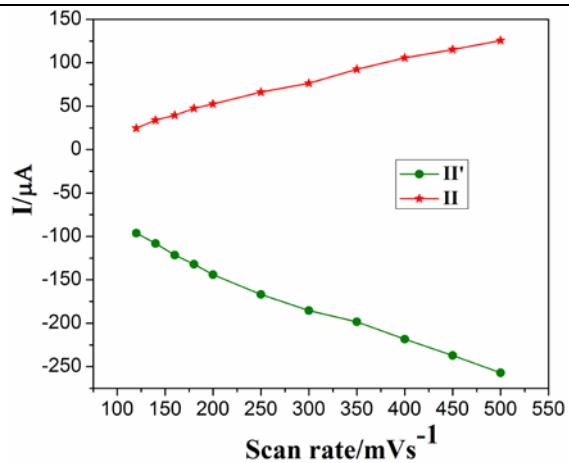


Figure S14. The dependence of cathodic peak (II) and anodic peak (II') currents of 2-CPE on scan rates.

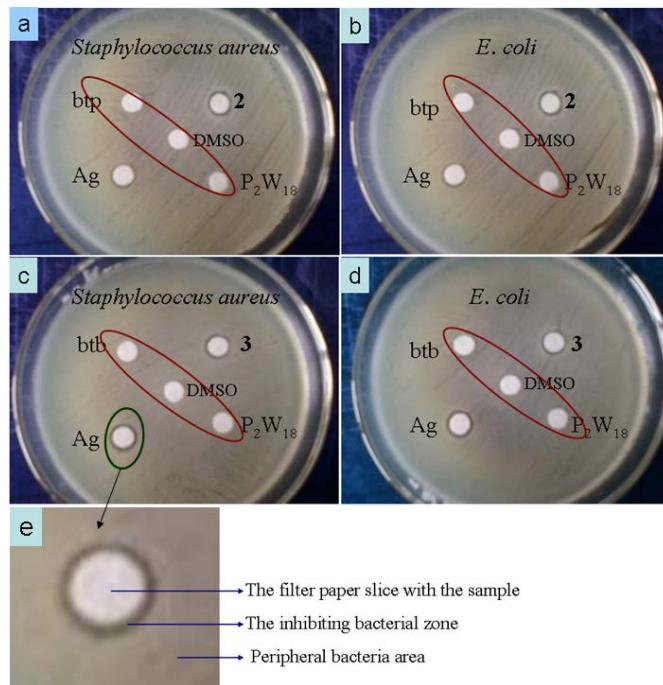


Figure S15. Optical photographs of antibacterial tests of compounds **2** and **3**, organic ligand btp and btb, materials dimethyl sulfoxide (DMSO), AgNO_3 (Ag) and $\alpha\text{-K}_6\text{P}_2\text{W}_{18}\text{O}_{62}\cdot15\text{H}_2\text{O}$ (P_2W_{18}) against *Staphylococcus aureus* (a, c) and *E. coli* (b, d). (e) Detailed instructions for the antibacterial area.

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Table S1. Selected bond lengths (\AA) and bond angles ($^{\circ}$) for compounds **1–3**.

Compound 1			
O(53)-Ag(1)	2.595(2)	O(57)-Ag(1)	2.569(2)
O(50)-Ag(1)	2.867(3)	N(7)-Ag(1)	2.27(3)
N(1)-Ag(1)	2.225(17)	O(56)-Ag(2)	2.835(3)
N(17)-Ag(2)	2.16(18)	N(3)-Ag(2)	2.063(18)
O(49)-Ag(3)	2.849(2)	O(1W)-Ag(3)	2.581(3)
N(11)-Ag(3)	2.191(18)	N(12)-Ag(3)	2.173(17)
O(46)-Ag(4)	2.779(2)	N(22)-Ag(4)	2.22(4)
N(18)-Ag(4)	2.377(18)	N(13)-Ag(4)	2.157(17)
O(45)-Ag(5)	2.755(3)	O(56)-Ag(5)	2.815(2)
O(63)-Ag(5)	2.762(3)	N(20)-Ag(5)	2.073(18)
O(45)-Ag(6)	2.725(3)	O(63)-Ag(6)	2.70(3)
N(5)-N(6)	1.43(5)	N(24)-Ag(6)	2.146(18)
O(48)-Ag(7)	2.262(3)	O(60)-Ag(7)	2.11(3)
N(8)-Ag(7)	2.13(4)	Ag(7)-Ag(2)	3.064(10)
C(2)-N(1)-Ag(1)	127.1(13)	N(2)-N(1)-Ag(1)	124.6(13)
C(8)-N(7)-Ag(1)	124(3)	C(7)-N(7)-Ag(1)	125(3)
N(1)-Ag(1)-N(7)	171.3(11)	N(1)-Ag(1)-O(53)	94.0(8)
N(7)-Ag(1)-O(53)	79.5(10)	C(2)-N(3)-Ag(2)	127.6(14)
C(1)-N(3)-Ag(2)	124.4(14)	N(11)-Ag(3)-O(1W)	101.9(9)
N(12)-Ag(3)-O(1W)	93.3(9)	N(10)-N(11)-Ag(3)	133.5(13)
C(23)-N(11)-Ag(3)	117.6(13)	C(12)-N(12)-Ag(3)	123.8(14)
C(11)-N(12)-Ag(3)	126.7(14)	N(12)-Ag(3)-N(11)	140.8(10)
C(18)-N(18)-Ag(4)	129.5(13)	N(19)-N(18)-Ag(4)	122.5(13)
N(14)-N(13)-Ag(4)	123.2(14)	C(11)-N(13)-Ag(4)	128.4(14)
C(21)-N(22)-Ag(4)	135(3)	N(21)-N(22)-Ag(4)	122(3)
N(13)-Ag(4)-N(22)	143.1(12)	N(13)-Ag(4)-N(18)	112.9(9)
N(22)-Ag(4)-N(18)	102.9(11)	C(18)-N(20)-Ag(5)	125.0(14)
C(17)-N(20)-Ag(5)	126.9(14)	C(23)-N(24)-Ag(6)	135.8(14)
C(24)-N(24)-Ag(6)	115.7(14)	C(23)-N(24)-Ag(6)	135.8(14)
C(24)-N(24)-Ag(6)	115.7(14)	O(60)-Ag(7)-W(4)	25.3(7)
O(60)-W(4)-Ag(7)	31.3(8)	O(29)-W(4)-Ag(7)	101.6(8)

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O(17)-W(4)-Ag(7)	133.4(7)	O(58)-W(4)-Ag(7)	66.6(7)
O(5)-W(4)-Ag(7)	92.7(7)	O(6)-W(4)-Ag(7)	140.6(6)
Compound 2			
Ag(1)-O(14)	2.570(10)	Ag(1)-O(36)	2.694(9)
Ag(1)-N(4)	2.173(15)	Ag(1)-N(9)	2.212(16)
Ag(2)-O(22)	2.683(10)	Ag(2)-O(18)	2.790(9)
Ag(2)-N(1)	2.088(16)	Ag(2)-N(10)	2.139(16)
Ag(3)-N(5)	2.230(17)	Ag(3)-N(7)	2.14(2)
Ag(3)-Ag(8)	2.42(2)	Ag(4)-O(40)	2.415(12)
Ag(4)-N(12)	2.32(2)	Ag(4)-N(20)	2.265(18)
Ag(4)-O(32)	2.786(13)	Ag(5)-N(13)	2.158(15)
Ag(5)-O(11)	2.632(3)	Ag(5)-Ag(6)	3.082(2)
Ag(5)-N(30)	2.15(2)	Ag(6)-N(18)	2.192(15)
Ag(6)-O(36)	2.605(13)	Ag(6)-O(14)	2.745(9)
Ag(6)-N(19)	2.150(15)	Ag(7)-N(24)	2.132(16)
Ag(7)-N(25)	2.129(17)	Ag(7)-O(17)	2.741(9)
Ag(8)-N(26)	2.343(16)	Ag(8)-O(29)	2.380(12)
Ag(8)-N(17)	2.803(9)	Ag(8)-O(55)	2.562(15)
N(4)-Ag(1)-N(9)	168.7(6)	N(9)-Ag(1)-O(14)	94.0(4)
N(1)-Ag(2)-N(10)	164.8(7)	N(7)-Ag(3)-N5	152.1(12)
N(12)-Ag(4)-O(40)	85.8(6)	N(13)-Ag(5)-N(30)	169.8(7)
N(19)-Ag(6)-N(18)	169.1(6)	N(19)-Ag(6)-O(36)	86.8(5)
N(25)-Ag(7)-N(24)	179.8(6)	N(26)-Ag(8)-O(55)	97.6(5)
Compound 3			
Ag(1)-N(12)	2.09(2)	Ag(1)-O(9)	2.446(14)
Ag(2)-O(47)	2.79(7)	Ag(2)-N(1)	2.08(2)
Ag(3)-O(35)	2.718(7)	Ag(3)-N(15)	2.07(2)
Ag(3)-N(19)	2.12(2)	Ag(4)-N(5)	2.142(18)
Ag(4)-N(11)	2.516(18)	Ag(4)-N(18)	2.156(19)
Ag(5)-O(28)	2.886(7)	Ag(5)-N(4)	2.178(18)
Ag(5)-N(7)	2.181(19)	Ag(5)-O(22)	2.613(7)
Ag(5)-O(22)	2.736(11)	N(12)-Ag(1)-O(9)	88.6(6)
C(15)-N(12)-Ag(1)	128.0(17)	C(16)-N(12)-Ag(1)	133.2(18)
N(1)-Ag(2)-N(1)	179.998(4)	C(2)-N(1)-Ag(2)	130.5(19)

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C(1)-N(1)-Ag(2)	128(2)	N(15)-Ag(3)-N(19)	164.4(11)
C(18)-N(15)-Ag(3)	130(2)	C(17)-N(15)-Ag(3)	123.5(17)
C(26)-N(19)-Ag(3)	123.6(19)	C(25)-N(19)-Ag(3)	130(2)
N(5)-Ag(4)-N(18)	161.2(7)	C(23)-N(18)-Ag(4)	125.8(16)
C(24)-N(18)-Ag(4)	130.5(16)	C(7)-N(5)-Ag(4)	129.5(15)
N(6)-N(5)-Ag(4)	129.3(14)	N(4)-Ag(5)-N(7)	160.9(8)
C(8)-N(4)-Ag(5)	127.7(15)	C(7)-N(4)-Ag(5)	125.6(17)
C(9)-N(7)-Ag(5)	124.2(17)	C(10)-N(7)-Ag(5)	124.9(15)