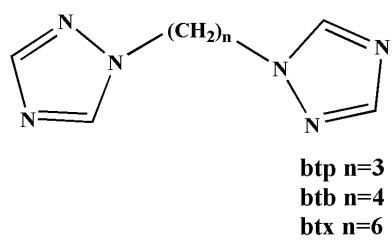


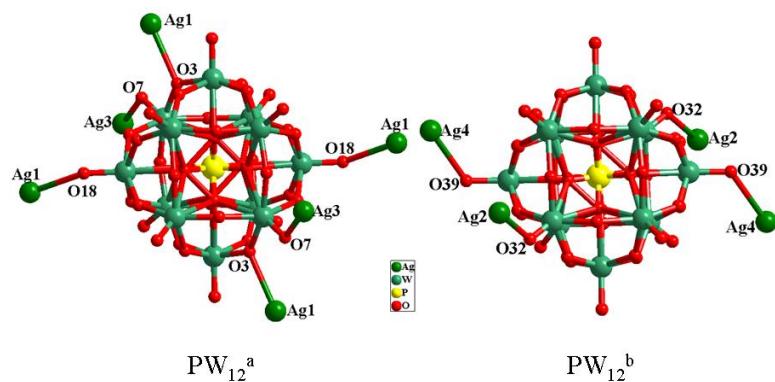
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A series of 3D  $\text{PW}_{12}\text{O}_{40}^{3-}$ -based  $\text{Ag}^{\text{I}}$ -bis(triazole) complexes containing different multinuclear loops: Syntheses, structures and properties †

Xiuli Wang,\* Dan Zhao, Aixiang Tian, \* and Jun Ying

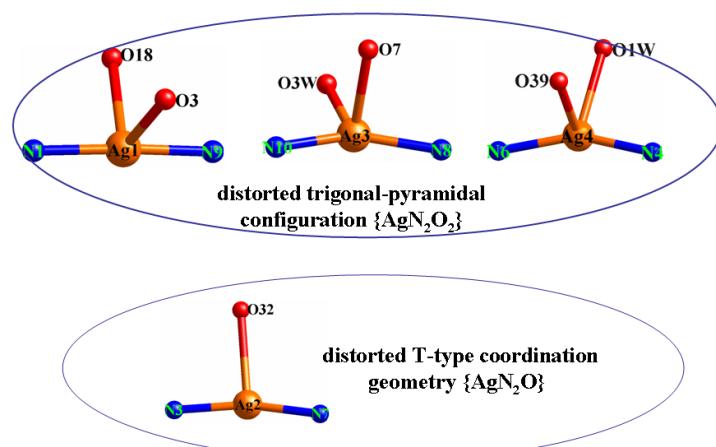


**Chart S1.** The organic ligands 1,3-bis(1,2,4-triazol-1-yl)ethane (btp), 1,4-bis(1,2,4-triazol-1-yl)butan (btb) and 1,6-bis(1,2,4-triazol-1-yl) hexane (btx) used in compounds **1–4**.

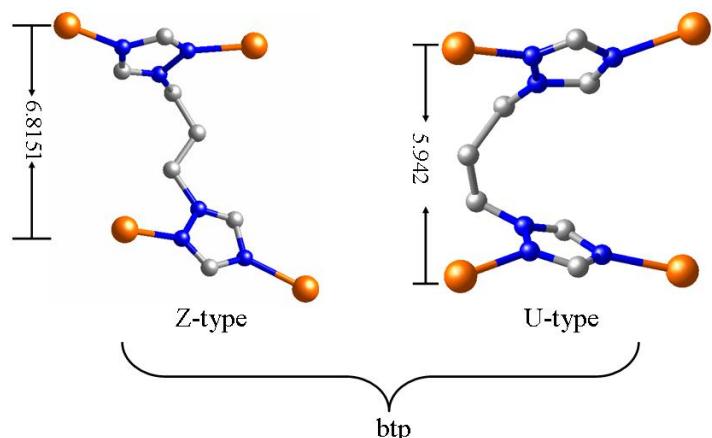


**Fig. S1** Two types of  $\text{PW}_{12}$  anions in compound **1** with different coordinated modes.

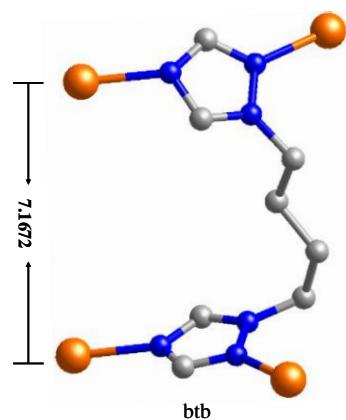
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**Fig. S2** The coordination environments and modes of four crystallographically independent  $\text{Ag}^{\text{I}}$  ions in compound 1.

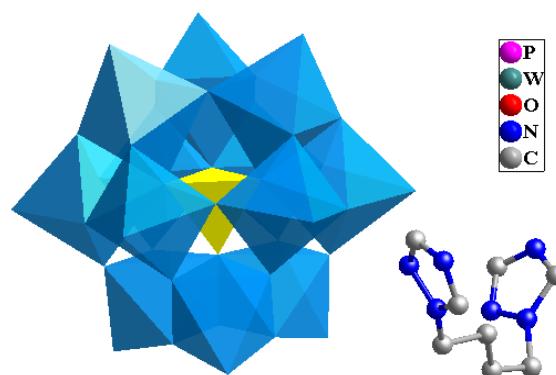


**Fig. S3** Two types of conformation modes and lengths of btp in compound 1

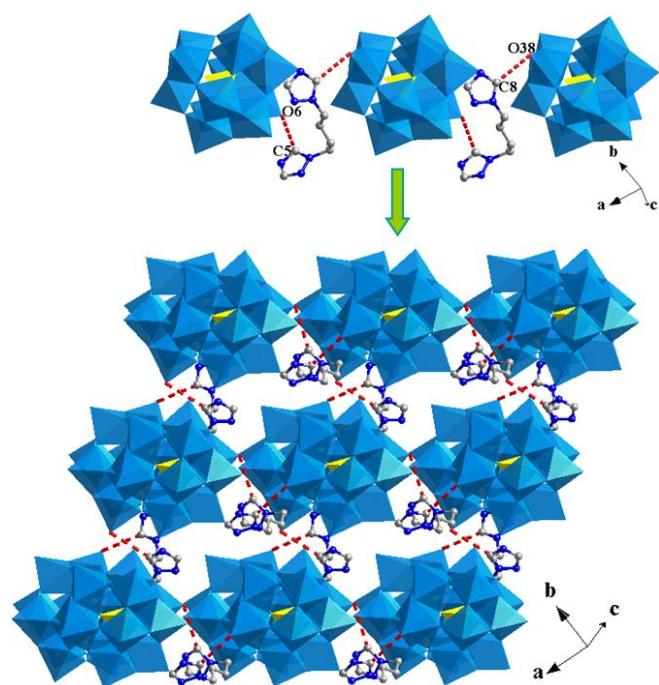


**Fig. S4** The conformation and coordination mode of btb in compound 2.

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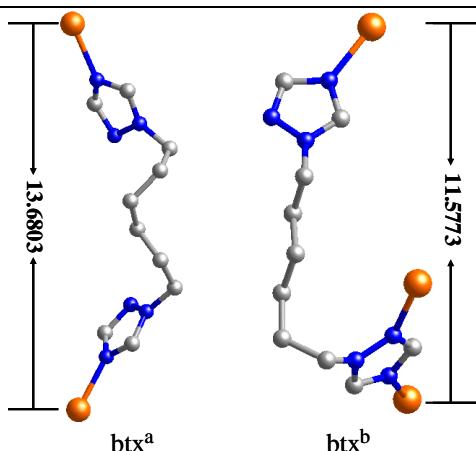


**Fig. S5** Ball/stick and polyhedral view of compound **3**. The hydrogen atoms and crystal water molecules are omitted for clarity.

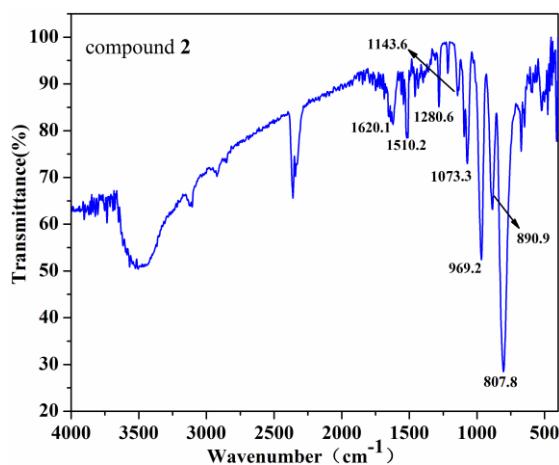
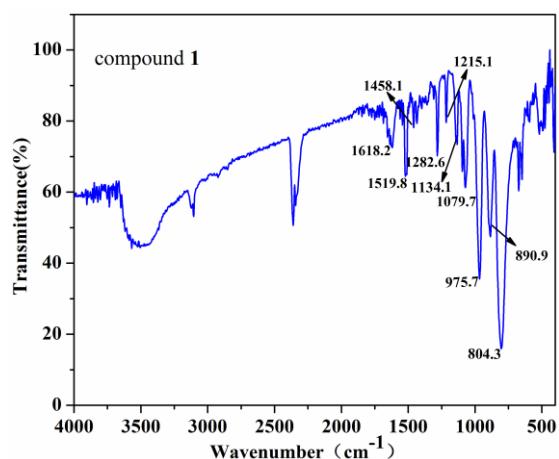


**Fig. S6** Ball/stick and polyhedral view of the supramolecular structure of compound **3**.

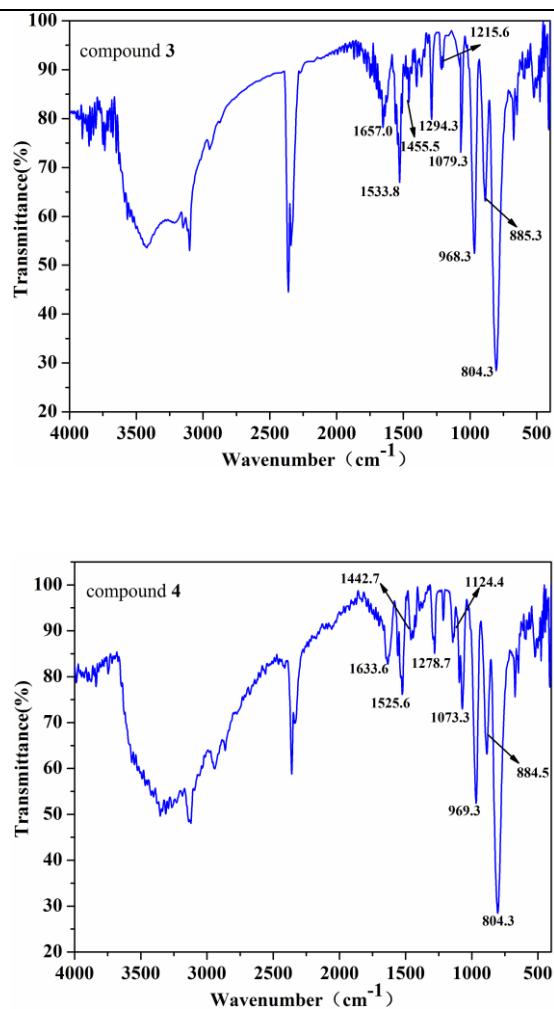
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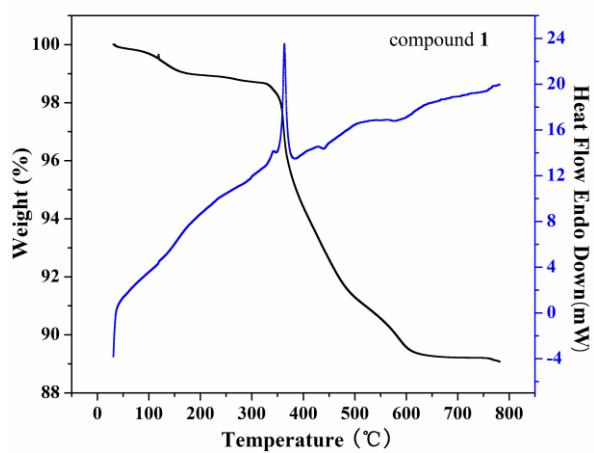
**Fig. S7** The two conformation and coordination modes ( $\text{btx}^{\text{a}}$  and  $\text{btx}^{\text{b}}$ ) and lengths of  $\text{btx}$  ligands in compound **4**.



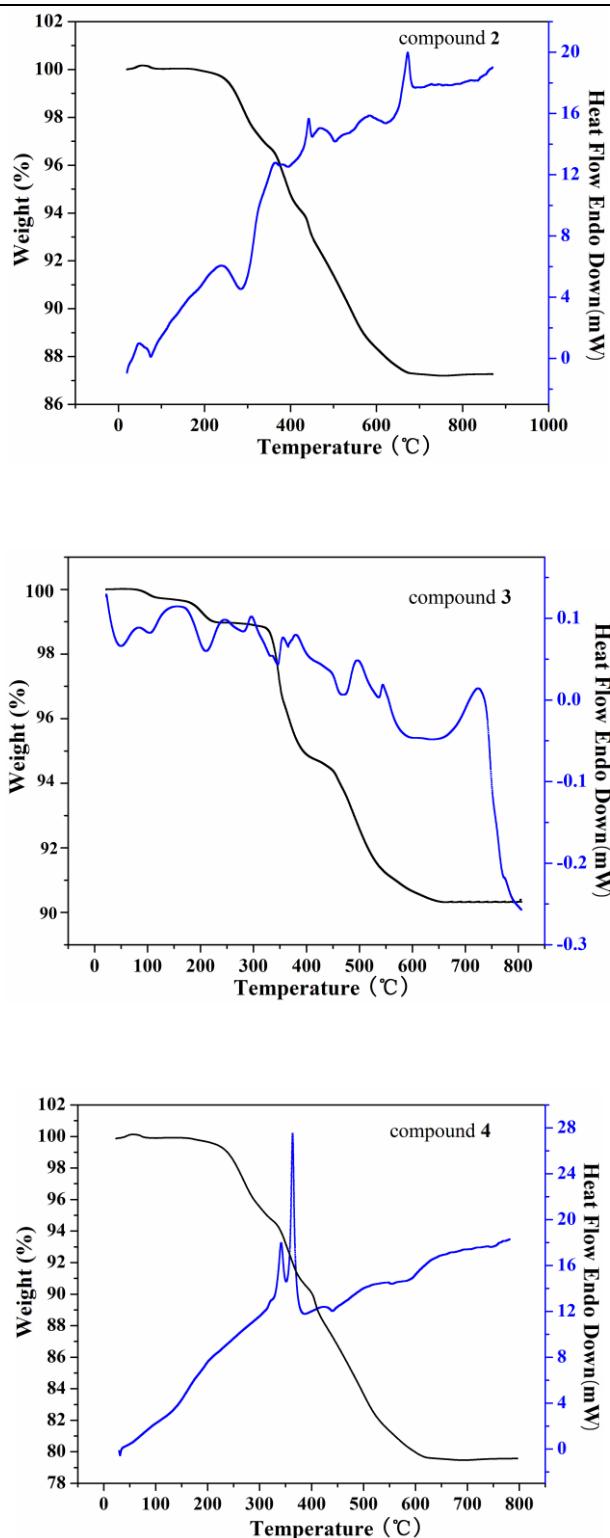
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**Fig. S8** The IR spectra of compounds 1–4.

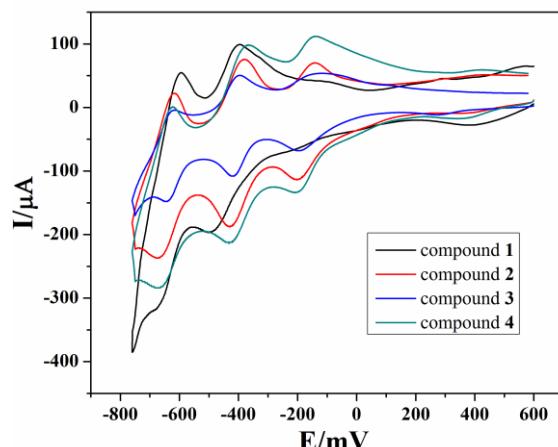


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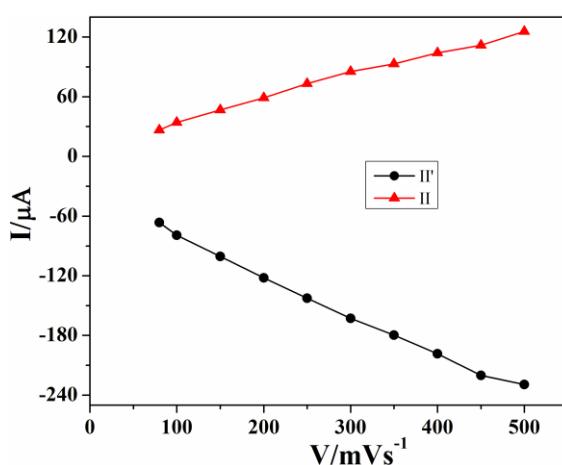


**Fig. S9** The TG curves of compounds 1–4.

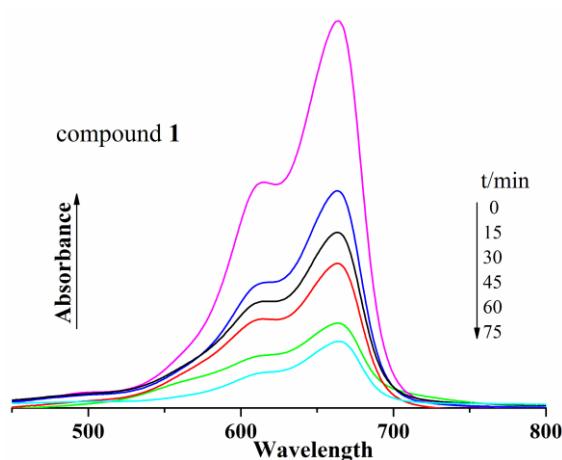
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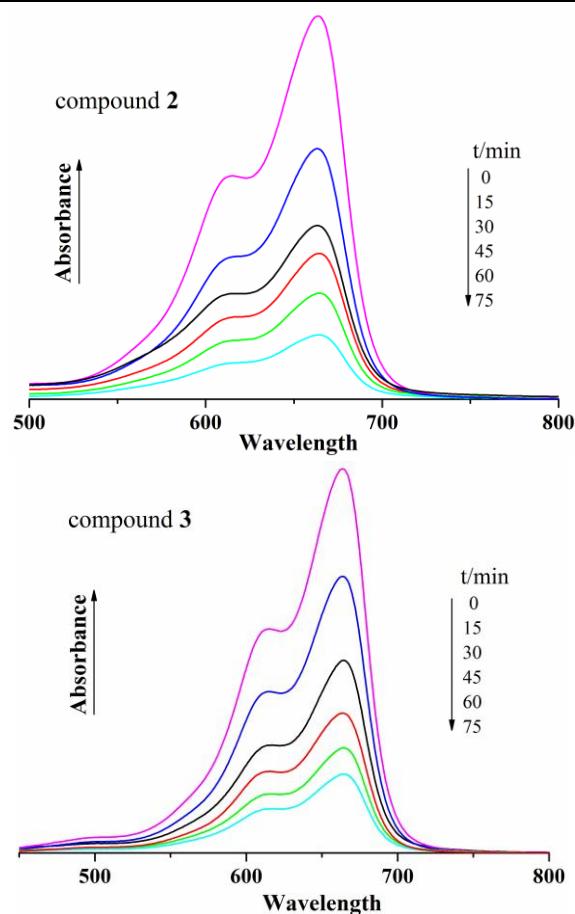
**Fig. S10** The cyclic voltammograms of the **1**–, **2**–, **3**– and **4**–CPEs in 0.5M  $\text{H}_2\text{SO}_4$  aqueous solution at scan rate of  $300 \text{ mV}\cdot\text{s}^{-1}$



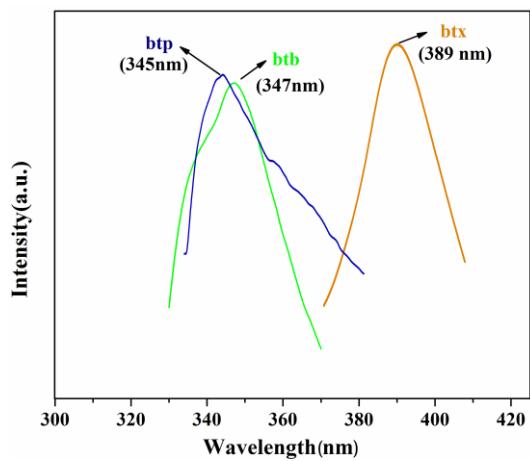
**Fig. S11** The dependence of cathodic peak (II) and anodic peak (II') currents of **1**–CPE on scan rates.



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**Fig. S12** Absorption spectra of the MB solution during the decomposition reaction under UV light irradiation with the use of **1**, **2** and **3**



**Fig. S13** The emission spectra of free ligands (blue: btp, green: btb, orange: btx).

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**Table S1** Selected bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) for compounds **1–4**.

| Compound 1          |           |                    |           |
|---------------------|-----------|--------------------|-----------|
| Ag(1)-N(1)          | 2.20(4)   | Ag(1)-N(9)         | 2.21(4)   |
| Ag(1)-O(3)          | 2.62(4)   | Ag(1)-O(18)        | 2.60(4)   |
| Ag(2)-N(3)          | 2.14(4)   | Ag(2)-N(7)#1       | 2.18(4)   |
| Ag(2)-O(32)         | 2.79(4)   | N(7)-Ag(2)#5       | 2.18(4)   |
| Ag(3)-O(7)          | 2.50(5)   | Ag(3)-O(3W)        | 2.31(4)   |
| Ag(3)-N(10)#2       | 2.18(4)   | Ag(3)-N(8)         | 2.22(4)   |
| N(10)-Ag(3)#6       | 2.18(4)   | Ag(4)-O(39)        | 2.74(4)   |
| Ag(4)-N(4)          | 2.17(4)   | Ag(4)-N(6)#3       | 2.24(4)   |
| N(1)-Ag(1)-N(9)     | 176.9(15) | C(7)-N(1)-Ag(1)    | 129(3)    |
| N(2)-N(1)-Ag(1)     | 125(3)    | C(12)-N(9)-Ag(1)   | 128(4)    |
| C(13)-N(9)-Ag(1)    | 126(3)    | O(18)-Ag(1)-N(9)   | 87.92(4)  |
| O(18)-Ag(1)-N(1)    | 93.96(3)  | O(3)-Ag(1)-N(9)    | 83.71(4)  |
| O(3)-Ag(1)-O(18)    | 97.38(3)  | N(3)-Ag(2)-N(7)#1  | 160.6(16) |
| C(1)-N(3)-Ag(2)     | 130(3)    | N(5)-N(3)-Ag(2)    | 127(3)    |
| C(14)-N(7)-Ag(2)#5  | 132(4)    | N(11)-N(7)-Ag(2)#5 | 121(3)    |
| O(32)-Ag(2)-N(7)    | 102.29(3) | O(32)-Ag(2)-N(3)   | 90.6(3)   |
| O(3W)-Ag(3)-N(10)#2 | 99.0(14)  | O(3W)-Ag(3)-N(8)   | 106.9(14) |
| N(10)#2-Ag(3)-N(8)  | 153.9(15) | O(3W)-Ag(3)-O(7)   | 87.3(15)  |
| C(12)-N(8)-Ag(3)    | 131(3)    | C(12)-N(9)-C(13)   | 120(3)    |
| N(10)#2-Ag(3)-O(7)  | 91.8(15)  | N(8)-Ag(3)-O(7)    | 93.0(15)  |
| C(6)-N(10)-Ag(3)#6  | 126(3)    | C(7)-N(10)-Ag(3)#6 | 130(4)    |
| W(12)-O(7)-Ag(3)    | 122(2)    | N(4)-Ag(4)-N(6)#3  | 155.0(16) |
| C(2)-N(4)-Ag(4)     | 125(3)    | C(1)-N(4)-Ag(4)    | 131(4)    |
| C(10)-N(6)-Ag(4)#4  | 129(3)    | C(14)-N(6)-Ag(4)#4 | 123(3)    |
| O(39)-Ag(4)-N(4)    | 93.69(3)  | O(39)-Ag(4)-N(6)   | 90.32(3)  |

Symmetry codes for **1**: #1 x+1, y-1, z #2 x, y+1, z #3 x+1, y, z #4 x-1, y, z #5 x-1, y+1, z #6 x, y-1, z #7 -x+1, -y, -z+1 #8 -x+2, -y+1, -z

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| Compound 2   |           |                   |           |
|--|-----------|-------------------|-----------|
| N(1)-Ag(1)   | 2.216(12) | N(4)-Ag(1)        | 2.215(12) |
| O(22)-Ag(1)  | 2.506(14) | Ag(1)-O(19)       | 2.807(12) |
| Ag(2)-O(17)  | 2.848(12) | N(3)-Ag(2)        | 2.141(12) |
| N(6)-Ag(2)#3   | 2.162(12) | Ag(2)-N(6)#5      | 2.162(12) |
| Ag(2)-O(19)  | 2.704(12) | N(1)-Ag(1)-O(19)  | 119.49(9) |
| C(2)-N(1)-Ag(1)  | 128.9(11) | N(2)-N(1)-Ag(1)   | 127.3(9)  |
| C(5)-N(4)-Ag(1)  | 125.3(11) | N(5)-N(4)-Ag(1)   | 131.9(9)  |
| W(1)-O(22)-Ag(1)   | 135.2(8)  | N(4)-Ag(1)-N(1)   | 152.6(5)  |
| N(4)-Ag(1)-O(22)   | 110.7(5)  | N(1)-Ag(1)-O(22)  | 82.8(5)   |
| Ag(1)-O(19)-Ag(2)  | 91.70(5)  | N(4)-Ag(1)-O(19)  | 85.06(5)  |
| C(1)-N(3)-Ag(2)  | 117.9(10) | C(2)-N(3)-Ag(2)   | 131.3(10) |
| C(4)-N(6)-Ag(2)#3  | 131.8(11) | C(5)-N(6)-Ag(2)#3 | 124.1(10) |
| N(3)-Ag(2)-N(6)#5  | 167.0(5)  | N(2)-Ag(2)-O(18)  | 96.78(5)  |
| N(3)-Ag(2)-O(19)   | 97.02(5)  | N(6)-Ag(2)-O(19)  | 95.32(5)  |
| O(17)-Ag(2)-N(3)   | 79.39(5)  | O(17)-Ag(2)-N(6)  | 92.87(5)  |
| Symmetry codes for 2: #1 x-1, -y+1/2, z-1/2 #2 x+1, -y+1/2, z+1/2 #3 -x+2, y+1/2, -z+1/2 #4 -x+2, -y, -z+1<br>#5 -x+2, y-1/2, -z+1/2 |           |                   |           |

| Compound 3 |           |            |           |
|------------|-----------|------------|-----------|
| P(1)-O(30) | 1.513(13) | P(1)-O(2)  | 1.519(17) |
| P(1)-O(29) | 1.537(17) | P(1)-O(37) | 1.540(14) |
| W(1)-O(31) | 1.717(15) | W(1)-O(33) | 1.877(13) |
| W(1)-O(27) | 1.891(15) | W(1)-O(4)  | 1.901(14) |
| W(1)-O(16) | 1.942(15) | W(1)-O(37) | 2.45(2)   |
| W(2)-O(6)  | 1.727(12) | W(2)-O(28) | 1.860(14) |
| W(2)-O(16) | 1.895(18) | W(2)-O(23) | 1.922(17) |
| W(2)-O(21) | 1.950(14) | W(2)-O(37) | 2.416(15) |
| W(3)-O(19) | 1.693(18) | W(3)-O(4)  | 1.895(12) |
| W(3)-O(12) | 1.915(15) | W(3)-O(32) | 1.922(15) |

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|                  |           |                  |           |
|------------------|-----------|------------------|-----------|
| W(3)-O(34)       | 1.936(14) | W(3)-O(30)       | 2.452(14) |
| W(4)-O(22)       | 1.717(16) | W(4)-O(15)       | 1.861(17) |
| W(4)-O(8)        | 1.873(12) | W(4)-O(32)       | 1.908(19) |
| W(4)-O(28)       | 1.940(12) | W(4)-O(30)       | 2.439(13) |
| W(5)-O(24)       | 1.708(16) | W(5)-O(23)       | 1.896(14) |
| W(5)-O(35)       | 1.904(16) | W(5)-O(15)       | 1.921(15) |
| W(5)-O(39)       | 1.956(14) | W(5)-O(2)        | 2.444(14) |
| W(6)-O(38)       | 1.710(12) | W(6)-O(7)        | 1.912(15) |
| W(6)-O(10)       | 1.914(18) | W(6)-O(26)       | 1.956(19) |
| W(6)-O(29)       | 2.429(13) | W(7)-O(3)        | 1.681(14) |
| W(7)-O(21)       | 1.889(13) | W(7)-O(40)       | 1.896(13) |
| W(7)-O(13)       | 1.903(18) | W(7)-O(27)       | 1.915(18) |
| W(7)-O(37)       | 2.417(15) | W(8)-O(25)       | 1.713(18) |
| W(8)-O(12)       | 1.886(15) | W(8)-O(36)       | 1.892(18) |
| W(8)-O(26)       | 1.895(14) | W(8)-O(33)       | 1.924(12) |
| W(8)-O(29)       | 2.42(2)   | W(10)-O(11)      | 1.937(17) |
| W(9)-O(1)        | 1.681(12) | W(10)-O(36)      | 1.97(2)   |
| W(9)-O(34)       | 1.874(17) | W(10)-O(29)      | 2.452(16) |
| W(9)-O(7)        | 1.910(15) | W(11)-O(17)      | 1.633(16) |
| W(9)-O(14)       | 1.93(2)   | W(11)-O(39)      | 1.873(17) |
| W(9)-O(8)        | 1.950(12) | W(11)-O(14)      | 1.880(18) |
| W(9)-O(30)       | 2.442(11) | W(11)-O(10)      | 1.883(17) |
| W(10)-O(5)       | 1.716(18) | W(11)-O(18)      | 1.942(18) |
| W(10)-O(40)      | 1.910(13) | W(11)-O(2)       | 2.426(13) |
| W(10)-O(20)      | 1.913(14) | W(12)-O(9)       | 1.716(18) |
| W(12)-O(11)      | 1.886(15) | W(12)-O(35)      | 1.929(14) |
| W(12)-O(13)      | 1.906(15) | W(12)-O(2)       | 2.470(16) |
| W(12)-O(18)      | 1.923(15) | O(37)-P(1)-O(2)  | 111.4(9)  |
| O(37)-P(1)-O(30) | 108.4(8)  | O(31)-W(1)-O(27) | 101.4(6)  |

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|                  |          |                  |          |
|------------------|----------|------------------|----------|
| O(2)-P(1)-O(30)  | 109.8(8) | O(33)-W(1)-O(27) | 91.6(5)  |
| O(37)-P(1)-O(29) | 109.4(8) | O(4)-W(1)-O(27)  | 156.4(7) |
| O(2)-P(1)-O(29)  | 110.3(8) | O(31)-W(1)-O(16) | 103.4(6) |
| O(30)-P(1)-O(29) | 107.5(8) | O(33)-W(1)-O(16) | 155.2(7) |
| O(31)-W(1)-O(33) | 101.4(6) | O(4)-W(1)-O(16)  | 89.0(5)  |
| O(31)-W(1)-O(4)  | 102.2(6) | O(27)-W(1)-O(16) | 83.8(6)  |
| O(33)-W(1)-O(4)  | 85.6(5)  | O(31)-W(1)-O(37) | 171.8(5) |
| O(33)-W(1)-O(37) | 83.9(6)  | O(16)-W(2)-O(23) | 155.7(5) |
| O(4)-W(1)-O(37)  | 84.4(6)  | O(28)-W(2)-O(23) | 85.3(6)  |
| O(27)-W(1)-O(37) | 72.0(5)  | O(6)-W(2)-O(21)  | 103.8(5) |
| O(16)-W(1)-O(37) | 71.4(5)  | O(16)-W(2)-O(21) | 86.9(6)  |
| O(6)-W(2)-O(16)  | 100.6(6) | O(28)-W(2)-O(21) | 155.2(4) |
| O(6)-W(2)-O(28)  | 100.8(5) | O(23)-W(2)-O(21) | 86.0(6)  |
| O(16)-W(2)-O(28) | 91.5(6)  | O(6)-W(2)-O(37)  | 172.1(6) |
| O(6)-W(2)-O(23)  | 103.6(7) | O(16)-W(2)-O(37) | 72.8(5)  |
| O(28)-W(2)-O(37) | 84.0(5)  | O(4)-W(3)-O(34)  | 156.1(7) |
| O(23)-W(2)-O(37) | 82.9(5)  | O(19)-W(3)-O(12) | 103.1(7) |
| O(21)-W(2)-O(37) | 71.9(4)  | O(32)-W(3)-O(12) | 156.7(7) |
| O(19)-W(3)-O(32) | 100.2(6) | O(4)-W(3)-O(12)  | 84.9(5)  |
| O(19)-W(3)-O(4)  | 100.9(6) | O(34)-W(3)-O(12) | 88.5(5)  |
| O(32)-W(3)-O(4)  | 90.3(5)  | O(19)-W(3)-O(30) | 172.1(5) |
| O(19)-W(3)-O(34) | 103.0(6) | O(32)-W(3)-O(30) | 73.9(6)  |
| O(32)-W(3)-O(34) | 86.7(5)  | O(4)-W(3)-O(30)  | 84.6(6)  |
| O(34)-W(3)-O(30) | 71.7(6)  | O(22)-W(4)-O(32) | 101.4(7) |
| O(12)-W(3)-O(30) | 82.9(6)  | O(15)-W(4)-O(32) | 154.5(6) |
| O(22)-W(4)-O(15) | 103.9(7) | O(8)-W(4)-O(32)  | 87.8(6)  |
| O(22)-W(4)-O(8)  | 101.2(5) | O(28)-W(4)-O(32) | 87.6(6)  |
| O(15)-W(4)-O(8)  | 89.8(6)  | O(22)-W(4)-O(30) | 171.7(6) |
| O(22)-W(4)-O(28) | 101.9(5) | O(15)-W(4)-O(30) | 82.7(6)  |

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|                  |          |                  |          |
|------------------|----------|------------------|----------|
| O(15)-W(4)-O(28) | 84.7(6)  | O(8)-W(4)-O(30)  | 73.5(5)  |
| O(8)-W(4)-O(28)  | 156.9(5) | O(28)-W(4)-O(30) | 83.5(4)  |
| O(32)-W(4)-O(30) | 72.3(5)  | O(35)-W(5)-O(39) | 83.1(5)  |
| O(24)-W(5)-O(35) | 99.4(7)  | O(23)-W(5)-O(39) | 156.2(6) |
| O(24)-W(5)-O(23) | 104.0(6) | O(15)-W(5)-O(39) | 91.2(6)  |
| O(35)-W(5)-O(23) | 90.3(6)  | O(24)-W(5)-O(2)  | 168.9(6) |
| O(24)-W(5)-O(15) | 106.9(6) | O(35)-W(5)-O(2)  | 72.7(6)  |
| O(35)-W(5)-O(15) | 153.7(6) | O(23)-W(5)-O(2)  | 84.1(5)  |
| O(23)-W(5)-O(15) | 84.7(6)  | O(15)-W(5)-O(2)  | 81.1(5)  |
| O(24)-W(5)-O(39) | 99.6(6)  | O(39)-W(5)-O(2)  | 72.1(5)  |
| O(38)-W(6)-O(10) | 106.7(6) | O(3)-W(7)-O(27)  | 101.8(6) |
| O(38)-W(6)-O(7)  | 100.9(5) | O(21)-W(7)-O(27) | 87.1(6)  |
| O(10)-W(6)-O(7)  | 84.2(6)  | O(3)-W(7)-O(40)  | 104.4(6) |
| O(38)-W(6)-O(20) | 103.8(5) | O(21)-W(7)-O(40) | 155.7(5) |
| O(10)-W(6)-O(20) | 91.4(6)  | O(27)-W(7)-O(40) | 90.4(6)  |
| O(7)-W(6)-O(20)  | 155.1(4) | O(3)-W(7)-O(13)  | 103.0(7) |
| O(38)-W(6)-O(26) | 97.9(6)  | O(21)-W(7)-O(13) | 89.1(6)  |
| O(10)-W(6)-O(26) | 155.0(5) | O(27)-W(7)-O(13) | 155.3(5) |
| O(7)-W(6)-O(26)  | 86.5(6)  | O(40)-W(7)-O(13) | 83.1(6)  |
| O(20)-W(6)-O(26) | 87.4(6)  | O(3)-W(7)-O(37)  | 170.4(5) |
| O(38)-W(6)-O(29) | 169.1(6) | O(21)-W(7)-O(37) | 73.0(5)  |
| O(10)-W(6)-O(29) | 83.7(5)  | O(27)-W(7)-O(37) | 72.0(5)  |
| O(7)-W(6)-O(29)  | 82.9(4)  | O(40)-W(7)-O(37) | 83.2(5)  |
| O(20)-W(6)-O(29) | 72.3(4)  | O(13)-W(7)-O(37) | 83.6(5)  |
| O(26)-W(6)-O(29) | 72.1(5)  | O(25)-W(8)-O(12) | 103.0(7) |
| O(3)-W(7)-O(21)  | 99.8(5)  | O(25)-W(8)-O(36) | 97.4(7)  |
| O(12)-W(8)-O(36) | 159.4(7) | O(1)-W(9)-O(14)  | 105.1(7) |
| O(25)-W(8)-O(26) | 102.2(6) | O(34)-W(9)-O(14) | 155.4(5) |
| O(12)-W(8)-O(26) | 90.2(5)  | O(7)-W(9)-O(14)  | 83.7(6)  |

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|                   |          |                   |          |
|-------------------|----------|-------------------|----------|
| O(36)-W(8)-O(26)  | 88.9(6)  | O(1)-W(9)-O(8)    | 102.8(5) |
| O(25)-W(8)-O(33)  | 102.8(6) | O(34)-W(9)-O(8)   | 87.0(6)  |
| O(12)-W(8)-O(33)  | 84.5(5)  | O(7)-W(9)-O(8)    | 155.6(5) |
| O(36)-W(8)-O(33)  | 87.7(5)  | O(14)-W(9)-O(8)   | 89.2(6)  |
| O(26)-W(8)-O(33)  | 155.0(7) | O(1)-W(9)-O(30)   | 170.8(7) |
| O(25)-W(8)-O(29)  | 171.2(6) | O(34)-W(9)-O(30)  | 72.5(5)  |
| O(12)-W(8)-O(29)  | 84.6(6)  | O(7)-W(9)-O(30)   | 83.1(4)  |
| O(36)-W(8)-O(29)  | 75.4(6)  | O(14)-W(9)-O(30)  | 83.2(5)  |
| O(26)-W(8)-O(29)  | 73.1(5)  | O(8)-W(9)-O(30)   | 72.9(4)  |
| O(33)-W(8)-O(29)  | 82.1(5)  | O(5)-W(10)-O(40)  | 103.2(5) |
| O(1)-W(9)-O(34)   | 99.4(7)  | O(5)-W(10)-O(20)  | 100.1(5) |
| O(1)-W(9)-O(7)    | 101.6(5) | O(40)-W(10)-O(20) | 156.5(6) |
| O(34)-W(9)-O(7)   | 89.8(6)  | O(5)-W(10)-O(11)  | 104.8(7) |
| O(40)-W(10)-O(11) | 84.2(6)  | O(39)-W(11)-O(10) | 156.7(5) |
| O(20)-W(10)-O(11) | 87.0(6)  | O(17)-W(11)-O(18) | 100.0(6) |
| O(5)-W(10)-O(36)  | 99.7(7)  | O(14)-W(11)-O(18) | 157.4(6) |
| O(40)-W(10)-O(36) | 91.7(6)  | O(39)-W(11)-O(18) | 85.1(6)  |
| O(20)-W(10)-O(36) | 87.2(6)  | O(10)-W(11)-O(18) | 88.9(6)  |
| O(11)-W(10)-O(36) | 155.5(6) | O(17)-W(11)-O(2)  | 174.4(6) |
| O(5)-W(10)-O(29)  | 169.5(5) | O(14)-W(11)-O(2)  | 83.7(5)  |
| O(40)-W(10)-O(29) | 84.4(5)  | O(39)-W(11)-O(2)  | 74.6(5)  |
| O(20)-W(10)-O(29) | 72.9(5)  | O(10)-W(11)-O(2)  | 82.1(5)  |
| O(11)-W(10)-O(29) | 83.0(6)  | O(18)-W(11)-O(2)  | 74.7(5)  |
| O(36)-W(10)-O(29) | 72.5(5)  | O(9)-W(12)-O(11)  | 102.6(6) |
| O(17)-W(11)-O(14) | 101.8(6) | O(9)-W(12)-O(13)  | 103.0(6) |
| O(17)-W(11)-O(39) | 103.3(6) | O(11)-W(12)-O(13) | 85.6(6)  |
| O(14)-W(11)-O(39) | 95.8(6)  | O(9)-W(12)-O(35)  | 102.7(7) |
| O(17)-W(11)-O(10) | 99.9(6)  | O(11)-W(12)-O(35) | 154.7(7) |
| O(14)-W(11)-O(10) | 81.4(6)  | O(13)-W(12)-O(35) | 89.1(5)  |

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|                   |          |                   |          |
|-------------------|----------|-------------------|----------|
| O(9)-W(12)-O(18)  | 99.8(6)  | W(9)-O(7)-W(6)    | 150.9(9) |
| O(11)-W(12)-O(18) | 88.9(5)  | W(4)-O(8)-W(9)    | 125.8(7) |
| O(13)-W(12)-O(18) | 157.1(6) | W(6)-O(10)-W(11)  | 155.1(8) |
| O(35)-W(12)-O(18) | 86.5(5)  | W(12)-O(11)-W(10) | 151.4(7) |
| O(9)-W(12)-O(2)   | 171.5(6) | W(8)-O(12)-W(3)   | 151.7(7) |
| O(11)-W(12)-O(2)  | 82.7(6)  | W(12)-O(13)-W(7)  | 152.6(8) |
| O(13)-W(12)-O(2)  | 83.8(5)  | W(11)-O(14)-W(9)  | 155.2(8) |
| O(35)-W(12)-O(2)  | 72.2(6)  | W(4)-O(15)-W(5)   | 154.6(8) |
| O(18)-W(12)-O(2)  | 73.4(5)  | W(2)-O(16)-W(1)   | 127.2(7) |
| P(1)-O(2)-W(11)   | 128.2(7) | W(11)-O(18)-W(12) | 122.7(8) |
| P(1)-O(2)-W(12)   | 125.1(8) | W(10)-O(20)-W(6)  | 126.0(6) |
| W(11)-O(2)-W(12)  | 89.0(5)  | W(7)-O(21)-W(2)   | 126.4(6) |
| P(1)-O(2)-W(5)    | 125.4(7) | W(5)-O(23)-W(2)   | 151.3(8) |
| W(11)-O(2)-W(5)   | 88.6(5)  | W(8)-O(26)-W(6)   | 125.6(7) |
| W(12)-O(2)-W(5)   | 88.2(5)  | W(7)-O(27)-W(1)   | 128.2(7) |
| W(1)-O(4)-W(3)    | 150.1(7) | W(2)-O(28)-W(4)   | 151.3(8) |
| P(1)-O(29)-W(10)  | 124.8(8) | W(8)-O(36)-W(10)  | 122.7(7) |
| P(1)-O(29)-W(8)   | 127.7(8) | P(1)-O(37)-W(2)   | 127.0(8) |
| W(10)-O(29)-W(8)  | 89.3(5)  | P(1)-O(37)-W(1)   | 126.8(9) |
| P(1)-O(29)-W(6)   | 125.3(7) | W(2)-O(37)-W(1)   | 88.5(4)  |
| W(10)-O(29)-W(6)  | 88.7(4)  | P(1)-O(37)-W(7)   | 125.7(8) |
| W(8)-O(29)-W(6)   | 89.0(4)  | W(2)-O(37)-W(7)   | 88.3(4)  |
| P(1)-O(30)-W(3)   | 128.0(8) | W(1)-O(37)-W(7)   | 87.9(4)  |
| P(1)-O(30)-W(9)   | 126.4(7) | W(11)-O(39)-W(5)  | 124.7(8) |
| W(3)-O(30)-W(9)   | 88.6(5)  | W(10)-O(40)-W(7)  | 153.9(8) |
| P(1)-O(30)-W(4)   | 125.2(7) | W(9)-O(30)-W(4)   | 88.3(5)  |
| W(3)-O(30)-W(4)   | 87.7(4)  | W(9)-O(34)-W(3)   | 127.1(7) |
| W(3)-O(32)-W(4)   | 125.3(7) | W(5)-O(35)-W(12)  | 126.9(8) |
| W(1)-O(33)-W(8)   | 152.6(8) |                   |          |

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| Compound 4  |           |                     |           |
|---|-----------|---------------------|-----------|
| Ag(1)-N(9)  | 2.107(19) | Ag(1)-N(1)          | 2.16(2)   |
| Ag(1)-O(19)#1   | 2.568(14) | Ag(1)-O(21)         | 2.579(15) |
| O(19)-Ag(1)#6   | 2.568(14) | Ag(2)-N(4)          | 2.12(2)   |
| Ag(2)-N(12)#2   | 2.13(2)   | N(12)-Ag(2)#5       | 2.13(2)   |
| Ag(2)-O(18)   | 2.726(14) | Ag(2)#5-O(18)       | 2.726(14) |
| Ag(3)-N(6)#3  | 2.13(2)   | Ag(3)-N(6)          | 2.13(2)   |
| N(9)-Ag(1)-N(1)   | 167.1(8)  | N(9)-Ag(1)-O(19)#1  | 109.9(5)  |
| N(1)-Ag(1)-O(19)#1  | 82.1(7)   | N(9)-Ag(1)-O(21)    | 89.3(6)   |
| N(1)-Ag(1)-O(21)  | 87.1(8)   | O(19)#1-Ag(1)-O(21) | 126.0(6)  |
| C(5)-N(1)-Ag(1)   | 130(2)    | C(1)-N(1)-Ag(1)     | 124.9(18) |
| C(9)-N(9)-Ag(1)   | 125.8(16) | C(8)-N(9)-Ag(1)     | 128.9(16) |
| W(5)-O(19)-Ag(1)#6  | 147.1(9)  | W(2)-O(21)-Ag(1)    | 157.7(11) |
| N(4)-Ag(2)-N(12)#2  | 170.1(8)  | N(5)-N(4)-Ag(2)     | 134.5(17) |
| C(19)-N(4)-Ag(2)  | 122.6(17) | C(19)-N(12)-Ag(2)#5 | 122.8(19) |
| N2-Ag(2)-O(18)  | 96.78(17) | N(4)-Ag(2)-O18      | 91.17(17) |
| C(20)-N(12)-Ag(2)#5   | 131.9(19) | N(6)#3-Ag(3)-N(6)   | 180.0(10) |
| C(7)-N(6)-Ag(3)   | 126.7(16) | C(6)-N(6)-Ag(3)     | 125.2(16) |
| Symmetry codes for 4: #1 x-1, y, z #2 x, -y+1/2, z+1/2 #3 -x+1, -y-1, -z+1 #4 -x+2, -y, -z #5 x, -y+1/2, z-1/2 #6 x+1, y, z |           |                     |           |