Electronic Supporting Information (ESI)

Dinuclear Silver(I) Complexes for the Design of Metal-Ligand Networks Based on Triazolopyrimidines

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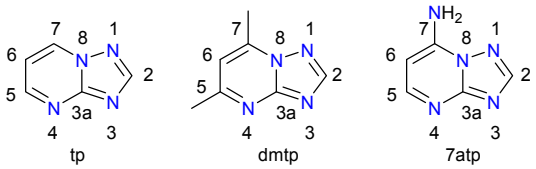

Scheme 1 1,2,4-Triazolo-[1,5-*a*]pyrimidine (tp) derivatives employed.

1. Thermogravimetric analysis of $\{[Ag_2(\mu_3\text{-tp})_2](PF_6)_2 \cdot \sim 6H_2O\}_n$ (6)

In case of the polymeric complex **6**, dehydration begins at room temperature so its TG and DSC diagrams (see Figure S1) were recorded immediately after taking crystals out of the solution. The percentage of weight loss is in good agreement with four water molecules per dimeric unit (8.87 %). Immediately after dehydration, an exothermic effect appears at 177 ºC, which probably indicates a structural change invoked by the loss of the water molecules embedded in the structure ($\Delta H = +16.4$ kJ mol^{-1}). At 297 ºC, an intense and well-defined endothermic effect appears, which is followed by the pyrolysis of the compound. This endothermic effect could be due to a melting process. Decomposition takes place in two steps and finishes at 950 ºC.

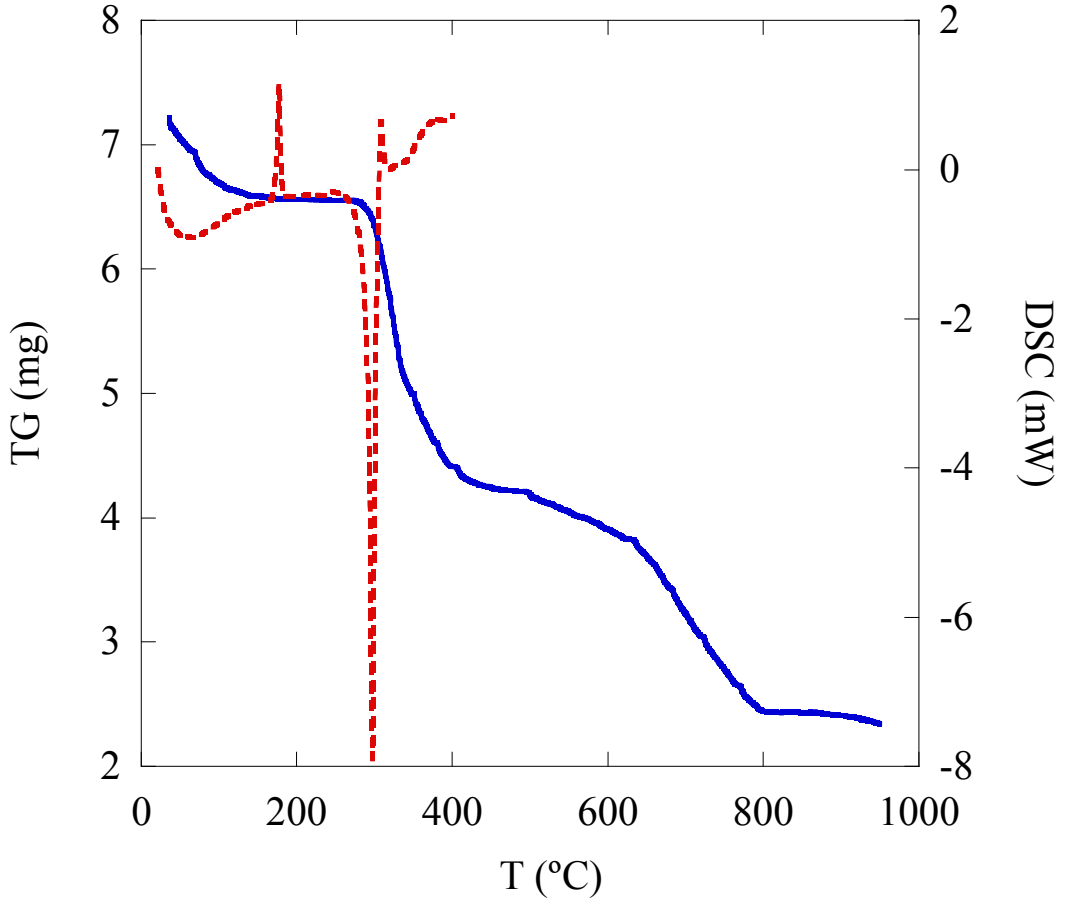

Fig. S1 TG / DSC plot of $\{[Ag_2(\mu_3\text{-tp})_2](PF_6)_2 \cdot \sim 6H_2O\}_n$ (**6**)

2. Supramolecular interactions in $[Ag_2(\mu\text{-}tp)_2(CH_3CN)_4](BF_4)_2$ (1)

Table S1

```
Ring-Metal Interactions with Cg-Me <   4.0 Ang.
================================================================================================================================

Cg(I) Res(I)   Me(J)    [   ARU(J)]  Cg(I)-Me(J) MeJ_Perp    Beta

Cg(2)  [ 1] -> Ag       [  2666.01]      3.599     3.344    21.73

[  2666] = 1-X,1-Y,1-Z

Ring 2 is N4-N8-C3A-C5-C6-C7

================================================================================================================================
Analysis of Short Non-Hydrogen Inter-Molecular Contacts For Inter-Molecular Clusters and/or Networks   (Minor Disorder Excluded)
================================================================================================================================

Contact-Nr Atom I[   ARU   ]      Atom J[   ARU   ]    d(I-J)   Del
--------------------------------------------------------------------------------------------------------------------------------
   1       Ag    [  1555.01] ...  C(5)  [  2666.01] =  3.411  -0.68
   2       Ag    [  1555.01] ...  C(6)  [  2666.01] =  3.430  -0.66


================================================================================================================================
Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg
================================================================================================================================
Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
================================================================================================================================

Nr Typ Res Donor --- H....Acceptor [    ARU  ]      D - H      H...A      D...A  D - H...A    A..H..A* A'..H..A" Sum(XY,YZ)  Sum(XZ)
--------------------------------------------------------------------------------------------------------------------------------

 1       1 C(7)  --H(71)  ..F(2)   [  2566.02]       0.95       2.45 3.0897(19)        125
 2       1 C(7)  --H(71)  ..N(1)   [  2676.01]       0.95       2.45   3.307(2)        150'        83'              358.00
 3       1 C(12) --H(121) ..F(4)   [  1554.02]       0.98       2.46   3.413(2)        165
 4       1 C(12) --H(122) ..F(2)   [  1654.02]       0.98       2.49   3.454(2)        170
 5       1 C(22) --H(222) ..F(4)   [  1554.02]       0.98       2.42   3.323(3)        152
 6       1 C(22) --H(223) ..F(2)   [  2556.02]       0.98       2.40   3.257(3)        145

:: No Classic Hydrogen Bonds Found


Translation of ARU-code to Equivalent Position Code
=====================================================
   [  2676. ]  = 1-x,2-y,1-z
   [  2566. ]  = -x,1-y,1-z
   [  1654. ]  = 1+x,y,-1+z
   [  1554. ]  = x,y,-1+z
   [  2556. ]  = -x,-y,1-z
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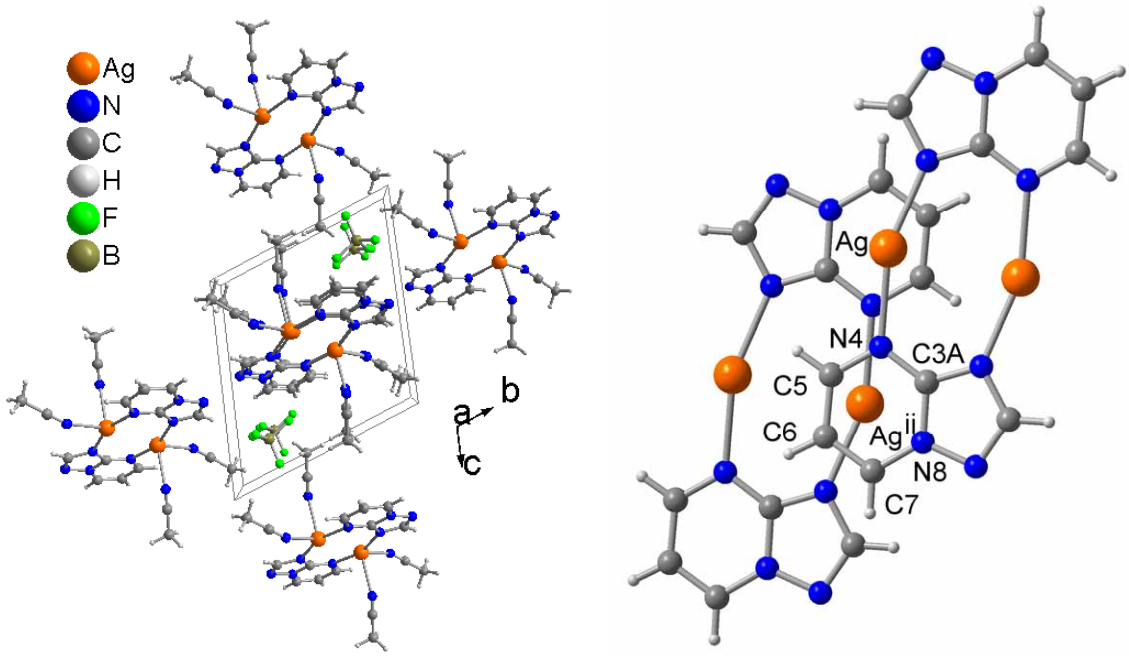

Fig. S2 Packing diagrams of $[Ag_2(tp)_2(CH_3CN)_4](BF_4)_2$ (**1**) with the Ag···π interaction at right; symmetry transformation ii = 1–x, 1–y, 1–z.

3. Supramolecular interactions in $[Ag_2(\mu\text{-}tp)_2(CH_3CN)_4](ClO_4)_2$ (2)

Table S2

```
Ring-Metal Interactions with Cg-Me <   4.0 Ang.
=================================================================================================================================

Cg(I) Res(I)   Me(J)    [   ARU(J)]  Cg(I)-Me(J) MeJ_Perp    Beta

Cg(2)  [ 1] -> Ag       [  2666.01]      3.631     3.328    23.57

[  2666] = 1-X,1-Y,1-Z

Ring 2 is N4-N8-C3A-C5-C6-C7

=================================================================================================================================
Analysis of Short Non-Hydrogen Inter-Molecular Contacts For Inter-Molecular Clusters and/or Networks   (Minor Disorder Excluded)
=================================================================================================================================

Contact-Nr Atom I[   ARU   ]      Atom J[   ARU   ]    d(I-J)   Del
---------------------------------------------------------------------------------------------------------------------------------
   1       Ag    [  1555.01] ...  C(5)  [  2666.01] =  3.414  -0.68
   2       Ag    [  1555.01] ...  C(6)  [  2666.01] =  3.413  -0.68


=================================================================================================================================
Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg
=================================================================================================================================
Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
=================================================================================================================================

Nr Typ Res Donor --- H....Acceptor [    ARU  ]      D - H      H...A      D...A  D - H...A    A..H..A* A'..H..A" Sum(XY,YZ)  Sum(XZ)
---------------------------------------------------------------------------------------------------------------------------------

 1       1 C(12) --H(12B) ..O(2)    [  1554.02]       0.98       2.57   3.455(5)        150
 2       1 C(12) --H(12C) ..O(1)    [  1654.02]       0.98       2.57   3.516(5)        162
 3       1 C(22) --H(22A) ..O(2)    [  1554.02]       0.98       2.54   3.293(5)        133
 4       1 C(22) --H(22B) ..O(1)    [  2556.02]       0.98       2.37   3.334(4)        167
 5       1 C(7)  --H(71)  ..O(1)    [  2566.02]       0.95       2.52   3.152(3)        124
 6       1 C(7)  --H(71)  ..N(1)    [  2676.01]       0.95       2.44   3.325(3)        155'        81'              360.00

:: No Classic Hydrogen Bonds Found


Translation of ARU-code to Equivalent Position Code
=====================================================
   [  2676. ]  = 1-x,2-y,1-z
   [  2566. ]  = -x,1-y,1-z
   [  1654. ]  = 1+x,y,-1+z
   [  1554. ]  = x,y,-1+z
   [  2556. ]  = -x,-y,1-z
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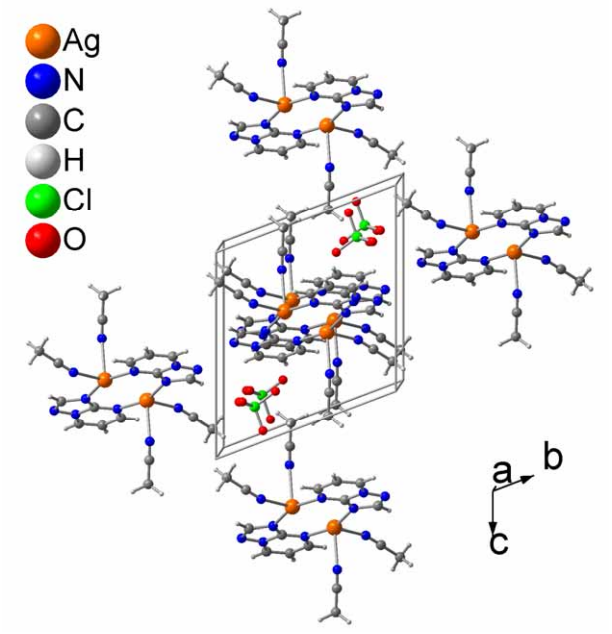

Fig. S3 Packing diagram of $[Ag_2(\mu\text{-}tp)_2(CH_3CN)_4](ClO_4)_2$ (**2**)

4. Supramolecular interactions in $[Ag_2(\mu\text{-}7atp)_2](ClO_4)_2$ (3)

Table S3

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================================================================================================================================================
Analysis of Short Ring-Interactions with Cg-Cg Distances <   6.0 Angstrom and Beta < 60.0 Deg.
================================================================================================================================================
- Cg(I)     = Plane number I (= ring number in () above)
- Alpha     = Dihedral Angle between Planes I and J (Deg)
- Beta      = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma     = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg     = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S  = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I) Res(I)   Cg(J)  [   ARU(J)]       Cg-Cg Transformed J-Plane P, Q, R, S     Alpha  Beta Gamma    CgI_Perp    CgJ_Perp  Slippage

Cg(1)  [ 1] -> Cg(1)  [  2566.01]    3.829(4) -0.5381-0.7160-0.4447  -1.5814         0 31.83 31.83   -3.253(2)   -3.253(2)   2.020
Cg(1)  [ 1] -> Cg(2)  [  2566.01]    3.890(4) -0.5583-0.6949-0.4532  -1.5592    1.7(3) 33.69 34.28   -3.214(2)   -3.236(2)
Cg(2)  [ 1] -> Cg(1)  [  2566.01]    3.889(4) -0.5381-0.7160-0.4447  -1.5814    1.7(3) 34.28 33.69   -3.236(2)   -3.214(2)
Cg(2)  [ 1] -> Cg(2)  [  2566.01]    4.885(3) -0.5583-0.6949-0.4532  -1.5592         0 48.51 48.51   -3.236(2)   -3.236(2)   3.659
                                  ----------                                  ------------------------------------------
                           Min or Max  3.829                                     0.00 31.83 48.51      -3.253      -3.253

[  2566] = -X,1-Y,1-Z

Ring 1 is N1-C2-N3-C3A-N8
Ring 2 is N4-N8-C3A-C5-C6-C7


Ring-Metal Interactions with Cg-Me <   4.0 Ang.
================================================================================================================================================

Cg(I) Res(I)   Me(J)   [   ARU(J)]  Cg(I)-Me(J) MeJ_Perp    Beta

Cg(1)  [ 1] -> Ag      [  1455.01]      3.683    -3.058    33.84
Cg(1)  [ 1] -> Ag      [  2566.01]      4.000    -3.309    34.18
Cg(2)  [ 1] -> Ag      [  2566.01]      3.558    -3.326    20.76

[  1455] = -1+X,Y,Z
[  2566] = -X,1-Y,1-Z


================================================================================================================================================
Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg
================================================================================================================================================
Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
================================================================================================================================================

Nr Typ Res Donor --- H....Acceptor [    ARU  ]      D - H      H...A      D...A  D - H...A    A..H..A* A'..H..A" Sum(XY,YZ)  Sum(XZ)
------------------------------------------------------------------------------------------------------------------------------------------------
 1       1 N(71) --H(71)  ..O(3)   [  1456.02]    0.84(9)   2.09(10)   2.913(8)    170(10)
 2 Intra 1 N(71) --H(72)  ..N(1)   [         ]   0.86(10)    2.37(9)   2.725(8)     105(8)
 3       1 N(71) --H(72)  ..O(2)   [  2576.02]   0.86(10)   2.23(10)   2.991(8)     147(8)'    108(4)'             360(12)

 4       1 C(2)  --H(2)   ..O(4)   [  1455.02]       0.93       2.50   3.229(7)        136
 5       1 C(6)  --H(6)   ..O(4)   [  1456.02]       0.93       2.60   3.516(7)        169

Translation of ARU-code to Equivalent Position Code
===================================================
   [  1456. ]  = -1+x,y,1+z
   [  2576. ]  = -x,2-y,1-z
   [  1455. ]  = -1+x,y,z
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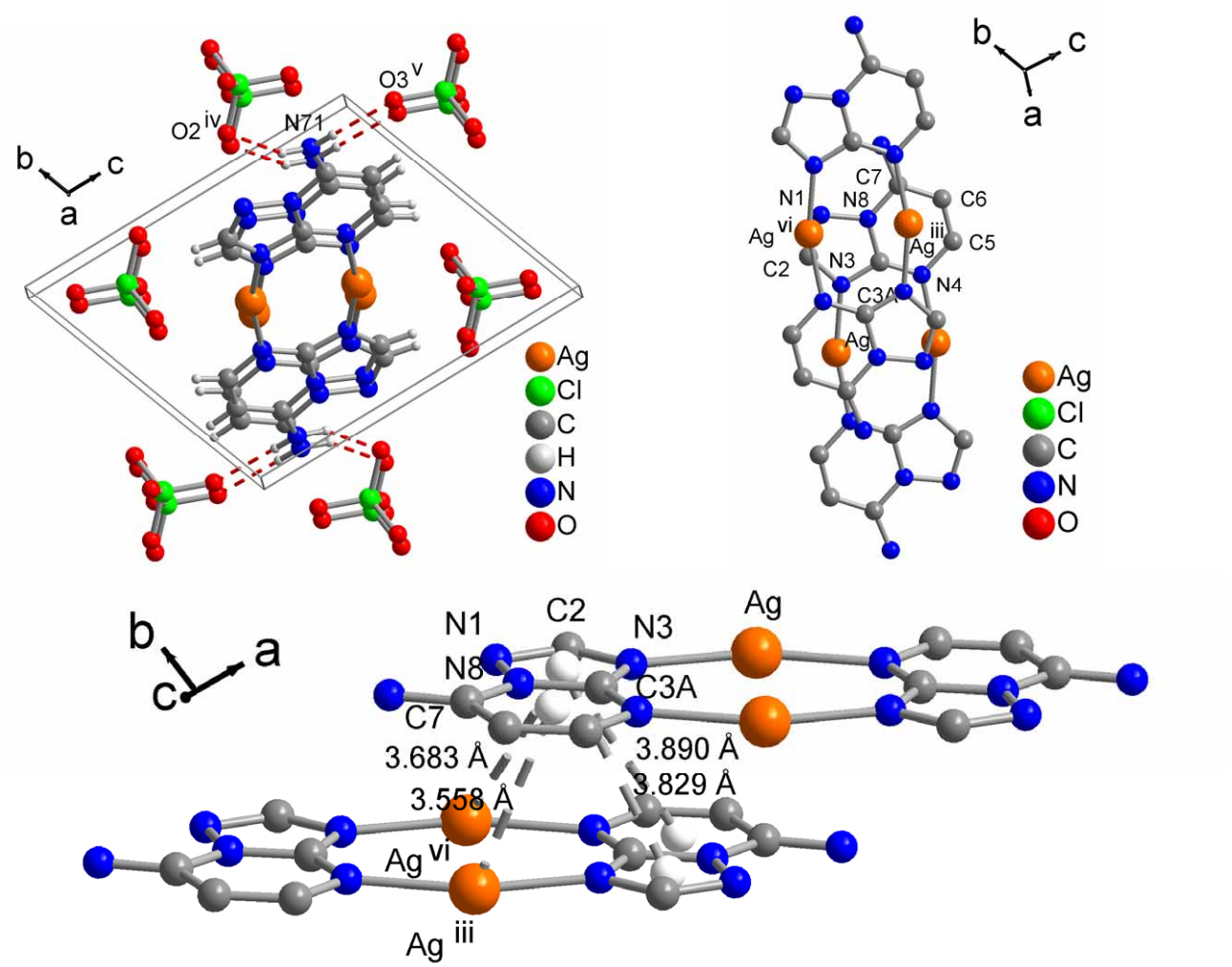

Fig. S4 Packing diagrams of $[Ag_2(\mu\text{-}7atp)_2](ClO_4)_2$ (**3**) with indication of the N-H···O hydrogen bonds at left and with the Ag···π and π···π interaction (distances in Å) at right and bottom; symmetry transformations iii = –x, 1–y, 1–z; iv = –x, 2–y, 1–z; ; v = –1+x, y, 1+z; vi = –1+x, y, z.

5. Supramolecular interactions in $[Ag_2(\mu\text{-dmtp})_2](PF_6)(ClO_4)$ (4)

Table S4

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================================================================================================================================
Analysis of Short Ring-Interactions with Cg-Cg Distances <   6.0 Angstrom and Beta < 60.0 Deg.
================================================================================================================================
- Cg(I)     = Plane number I (= ring number in () above)
- Alpha     = Dihedral Angle between Planes I and J (Deg)
- Beta      = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma     = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg     = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S  = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I) Res(I)   Cg(J)  [   ARU(J)]       Cg-Cg Transformed J-Plane P, Q, R, S     Alpha  Beta Gamma    CgI_Perp    CgJ_Perp  Slippage

Cg(1)   [ 1] -> Cg(2)  [  2656.01]    3.503(4)  0.3132-0.9458 0.0856   5.3711     5.4(3) 20.52 15.71   -3.372(2)    -3.281(3)
Cg(1)   [ 1] -> Cg(4)  [  1554.01]    5.973(4) -0.3295 0.9395-0.0939   1.7741     5.2(3) 54.50 49.44   -3.884(2)     3.468(2)
Cg(1)   [ 1] -> Cg(4)  [  2656.01]    3.664(4)  0.3295-0.9395 0.0939   5.4732     5.2(3) 23.05 23.37   -3.364(2)    -3.372(2)
Cg(2)   [ 1] -> Cg(1)  [  2656.01]    3.502(4)  0.3759-0.9265 0.0171   5.0823     5.4(3) 15.71 20.52   -3.281(3)    -3.371(2)
Cg(2)   [ 1] -> Cg(3)  [  1455.01]    5.603(4) -0.3740 0.9273-0.0132   2.0717     5.5(3) 47.98 46.60   -3.850(3)     3.751(2)
Cg(2)   [ 1] -> Cg(3)  [  2656.01]    3.745(4)  0.3740-0.9273 0.0132   5.0652     5.5(3) 26.31 28.65   -3.287(3)    -3.357(2)
Cg(3)   [ 1] -> Cg(2)  [  1655.01]    5.603(4) -0.3132 0.9458-0.0856  -5.7652     5.5(3) 46.60 47.98    3.751(2)    -3.850(3)
Cg(3)   [ 1] -> Cg(2)  [  2656.01]    3.745(4)  0.3132-0.9458 0.0856   5.3711     5.5(3) 28.65 26.31   -3.357(2)    -3.287(3)
Cg(3)   [ 1] -> Cg(4)  [  2656.01]    4.813(4)  0.3295-0.9395 0.0939   5.4732     5.3(3) 45.27 46.49   -3.313(2)    -3.387(2)
Cg(4)   [ 1] -> Cg(1)  [  1556.01]    5.974(4) -0.3759 0.9265-0.0171  -5.1787     5.2(3) 49.44 54.50    3.468(2)    -3.884(2)
Cg(4)   [ 1] -> Cg(1)  [  2656.01]    3.664(4)  0.3759-0.9265 0.0171   5.0823     5.2(3) 23.37 23.05   -3.372(2)    -3.363(2)
Cg(4)   [ 1] -> Cg(3)  [  2656.01]    4.813(4)  0.3740-0.9273 0.0132   5.0652     5.3(3) 46.49 45.27   -3.388(2)    -3.313(2)
Cg(4)   [ 1] -> Cg(4)  [  2667.01]    5.886(4)  0.3295-0.9395 0.0939  -1.6180          0 48.23 48.23    3.921(2)     3.922(2)   4.390
                                    ----------                                  ---------------------------------------------
                                Min or Max  3.502                                    0.03 15.71 54.50      -3.884       -3.884
```

Medium to strong π-π-stacking interactions are highlighted in blue. Strong π-stacking shows rather short centroid-centroid contacts (Cg···Cg < 3.8 Å) and small slip angles (β, γ< 25°) which translate into a sizable overlap of the aromatic planes. In comparison, π-stacking interactions can be viewed as medium to weak if they exhibit rather long centroid-centroid distances (Cg···Cg > 4.0 Å) together with large slip angles (β, γ> 30°).[1,2,3]

```
[  2656] = 1-X,-Y,1-Z
[  1554] = X,Y,-1+Z
[  1455] = -1+X,Y,Z
[  1655] = 1+X,Y,Z
[  1556] = X,Y,1+Z
[  2667] = 1-X,1-Y,2-Z

Ring 1 is N1-C2-N3-C3A-N8

Ring 2 is N11-C12-N13-C13A-N18

Ring 3 is N4-N8-C3A-C5-C6-C7

Ring 4 is N14-N18-C13A-C15-C16-C17

================================================================================================================================
Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg
================================================================================================================================
Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
================================================================================================================================

Nr Typ Res Donor --- H....Acceptor [    ARU  ]      D - H      H...A      D...A  D - H...A    A..H..A* A'..H..A" Sum(XY,YZ)  Sum(XZ)
--------------------------------------------------------------------------------------------------------------------------------

 1       1 C(2)  --H(2)   ..O(4)   [  2656.03]       0.93       2.39  3.068(11)        130
 2       1 C(6)  --H(6)   ..F(5)   [  1655.02]       0.93       2.48  3.376(11)        161
 3       1 C(9)  --H(9A)  ..F(4)   [         ]       0.96       2.41  3.237(13)        145
 4       1 C(16) --H(16)  ..F(3)   [  2667.02]       0.93       2.37   3.228(9)        153
 5 Intra 1 C(51) --H(51A) ..N(9)   [         ]       0.96       2.57  3.354(11)        139
 6       1 C(51) --H(51C) ..O(2)   [         ]       0.96       2.50  3.359(12)        149

:: No Classic Hydrogen Bonds Found


Translation of ARU-code to Equivalent Position Code
===================================================
   [  2656. ]  = 1-x,-y,1-z
   [  2667. ]  = 1-x,1-y,2-z
   [  1655. ]  = 1+x,y,z
```

1 C. Janiak, *J. Chem. Soc., Dalton Trans.* 2000, 3885.

2 H. Hosseini Monfared, M. Vahedpour, M. M. Yeganeh, M. Ghorbanloo, P. Mayer and C. Janiak, *Dalton Trans.*, 2011, **40**, 1286; H. A. Habib, A Hoffmann, H. A. Höppe, G. Steinfeld and C. Janiak, *Inorg. Chem.* 2009, **48**, 2166; B. Wu, X. Huang, Y. Xia, X.-J. Yang and C. Janiak, *CrystEngComm*, 2007, **9**, 676. B. Wisser and C. Janiak, *Acta Cryst.*, 2007, **E63**, o2871; T. Dorn, C. Janiak and K. Abu-Shandi, *CrystEngComm*, 2005, **7**, 633.

3 X.-J. Yang, F. Drepper, B. Wu, W.-H. Sun, W. Haehnel and C. Janiak, *Dalton Trans.*, 2005, 256; and supplementary material therein.

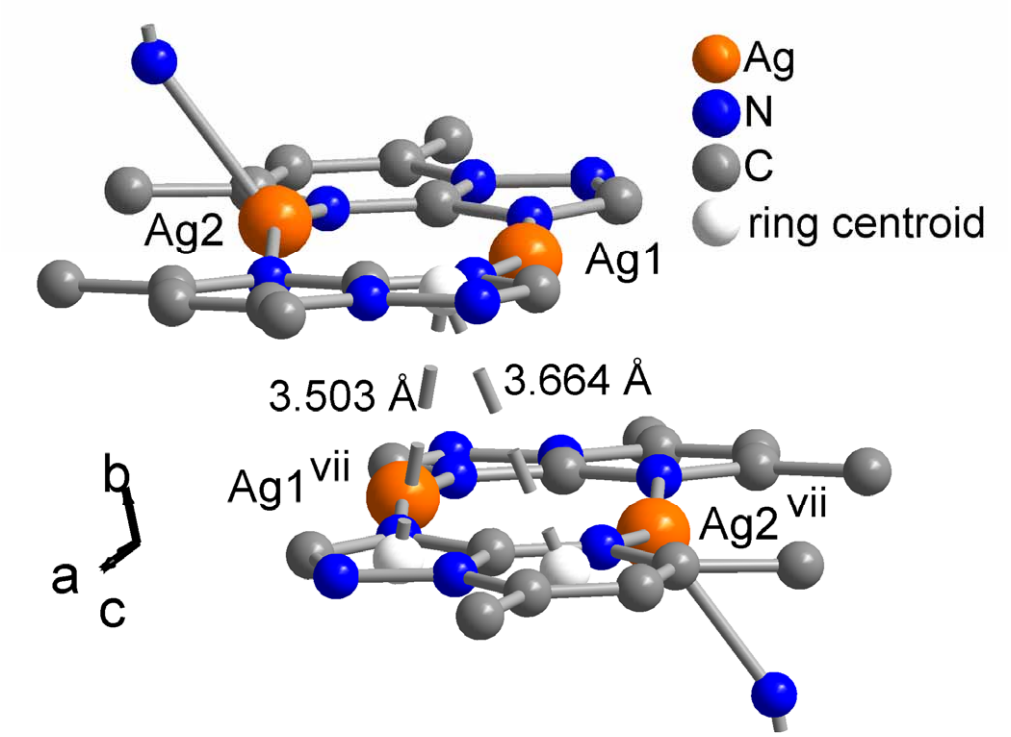


Fig. S5 Packing diagrams of $[Ag_2(\mu\text{-dmtp})_2](PF_6)(ClO_4)$ (**4**) with indication of the π···π interaction (distances in Å); symmetry transformations vii = 1–x, –y, 1–z

6. Supramolecular interactions in $[Ag_2(\mu\text{-}CF_3SO_3)_2(\mu\text{-}dmtp)_2]_n$ (5)

Table S5

```
================================================================================================================================================
Analysis of Short Ring-Interactions with Cg-Cg Distances <   6.0 Angstrom and Beta < 60.0 Deg.
================================================================================================================================================
- Cg(I)     = Plane number I (= ring number in () above)
- Alpha     = Dihedral Angle between Planes I and J (Deg)
- Beta      = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma     = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg     = Distance between ring Centroids (Ang.)
- CgI_Perp  = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp  = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage  = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S   = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I) Res(I)   Cg(J)  [   ARU(J)]       Cg-Cg Transformed J-Plane P, Q, R, S     Alpha  Beta Gamma    CgI_Perp    CgJ_Perp  Slippage

Cg(2)   [ 1] -> Cg(2)  [  2665.01]  3.5290(10) -0.7347 0.5292 0.4245  -1.3979          0 20.42 20.42   3.3072(7)   3.3073(7)   1.231

[  2665] = 1-X,1-Y,-Z

Ring 2 is N4-N8-C3A-C5-C6-C7
```

Medium to strong π-π-stacking interactions are highlighted in blue.

```
================================================================================================================================================
Analysis of Potential Hydrogen Bonds and Schemes with d(D...A) < R(D)+R(A)+0.50, d(H...A) < R(H)+R(A)-0.12 Ang., D-H...A > 100.0 Deg
================================================================================================================================================
Note: - ARU codes in [] are with reference to the Coordinates printed above (Possibly transformed, when MOVE .NE. 1.555)
================================================================================================================================================

Nr Typ Res Donor --- H....Acceptor [    ARU  ]      D - H      H...A      D...A  D - H...A    A..H..A* A'..H..A" Sum(XY,YZ)  Sum(XZ)
------------------------------------------------------------------------------------------------------------------------------------------------

 1       1 C(2)  --H(21)  ..F(11)  [  1655.01]       0.95       2.52   3.286(3)        138
 2 Intra 1 C(51) --H(51A) ..O(11)  [  2566.01]       0.98       2.46   3.381(2)        157
 3       1 C(51) --H(51B) ..F(11)  [  1545.01]       0.98       2.51   3.311(2)        139
 4       1 C(6)  --H(61)  ..O(13)  [  2565.01]       0.95       2.21   3.158(2)        173
 5       1 C(71) --H(71B) ..O(12)  [  1554.01]       0.98       2.42   3.292(2)        148

:: No Classic Hydrogen Bonds Found


Translation of ARU-code to Equivalent Position Code
===================================================
   [  2566. ]  = -x,1-y,1-z
   [  1545. ]  = x,-1+y,z
   [  2565. ]  = -x,1-y,-z
   [  1655. ]  = 1+x,y,z
   [  1554. ]  = x,y,-1+z
```

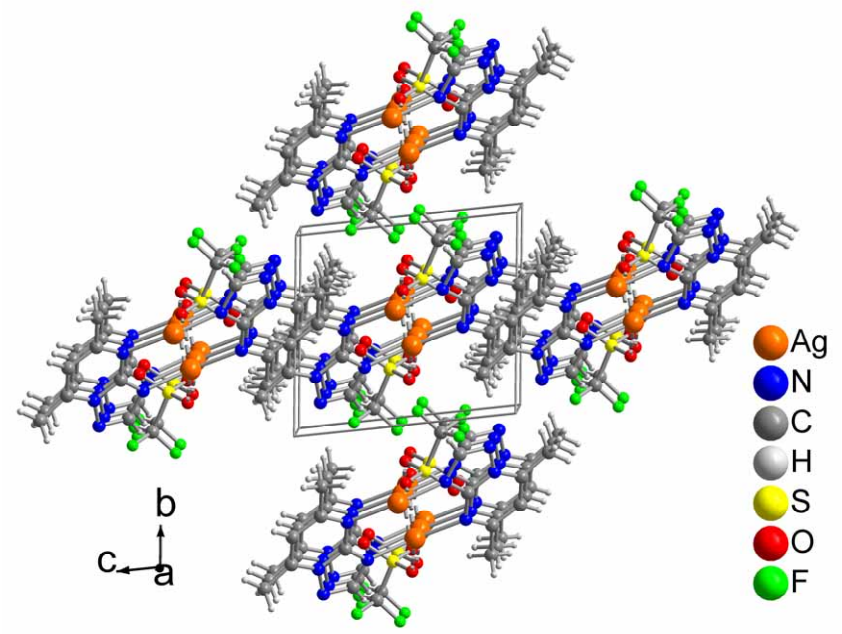
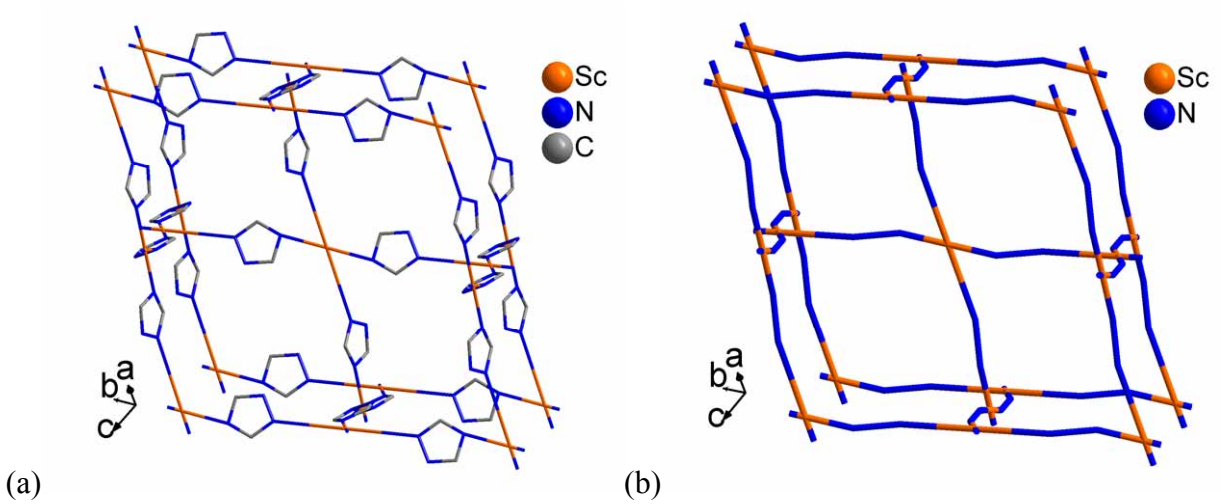


Fig. S6 Packing diagram of $[Ag_2(\mu\text{-}CF_3SO_3)_2(\mu\text{-}dmtp)_2]_n$ (**5**)

7. Net representations of $\{[Ag_2(\mu_3\text{-}tp)_2](PF_6)_2 \cdot \sim 6H_2O\}_n$ (6)



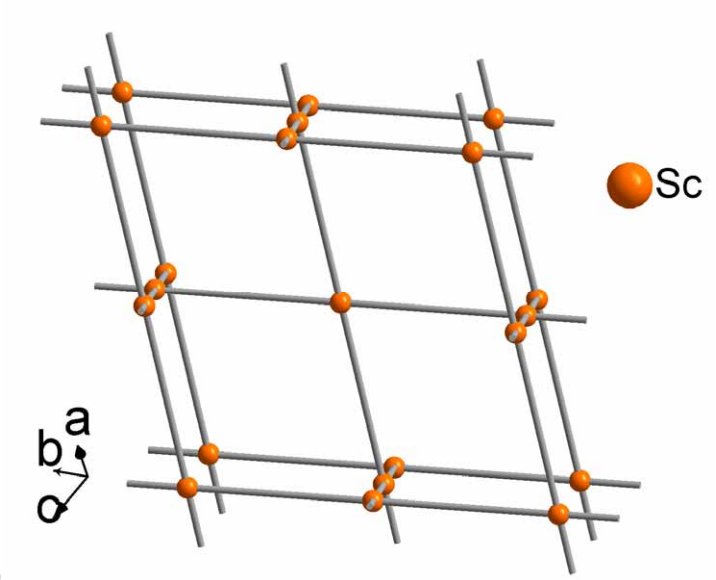


Fig. S7 Simplified net representation of **6** with the Ag···Ag midpoint (Sc) as the node. In (a) only the triazole ring of the ligand is shown for clarity and the Sc-node connected to N3 and N1. (b) and (c) represent further simplification to indication the NbO topology by shown only the Sc-N-N-Sc connectivity in (b) and only the Sc-Sc connectivity in (c).

8. Ag-Ag bond critical point in dinuclear complexes $Ag_2(\mu\text{-tp})_2$

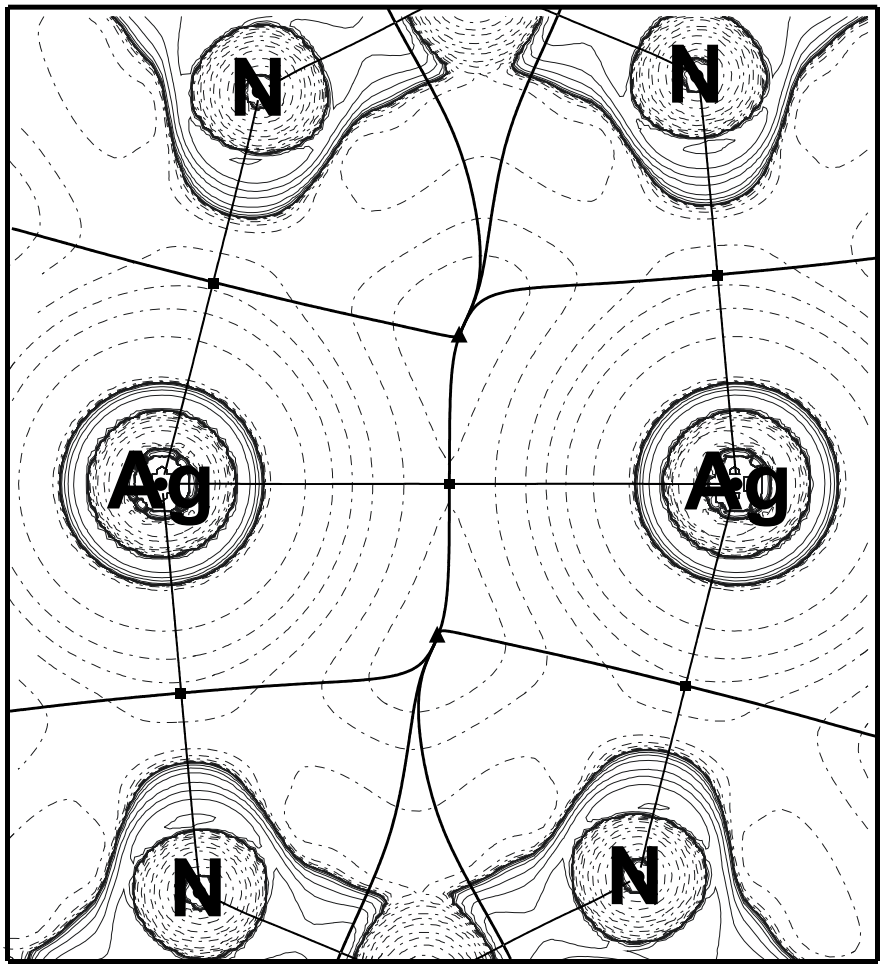


Fig. S8 Laplacian $\nabla^2\rho(r)$ contour map, in the molecular structure of $Ag_2(\mu\text{-tp})_2$ complex. The contour values correspond to ±0.02, ±0.04, ±0.08, ±0.2, ±0.4, ±0.8, ±2.0, ±4.0, and ±8.0 $e \cdot a_0^{-5}$, where the dashed lines indicate negative values.

9. Electronic basin populations of the ELF basins for the isolated ligands and complexes

Table S6

	tp	$Ag_2(\mu\text{-tp})_2$ complex	dmtp	$Ag_2(\mu\text{-dmtp})_2$ complex	7atp	$Ag_2(\mu\text{-7atp})_2$ complex
V(C3a,N1)	2.59	2.82	2.61	2.83	2.58	2.83
V(C3a,N3)	2.72	2.73	2.69	2.69	2.64	2.61
V(C3a,N8)	2.21	2.33	2.19	2.33	2.17	2.3
V(C5,N4)	2.55	2.51	2.57	2.46	2.44	2.29
V(C6,C5)	2.54	2.56	2.54	2.61	3.05	3.19
V(C7,C6)	3.21	1.60+1.50	3.30	3.15	2.85	2.61
V(C7,N8)	2.32	2.38	2.28	2.34	2.24	2.26
V(N1)	3.23	3.01	3.25	3.03	3.28	3.05
V(N3,C2)	2.28	2.16	2.27	2.16	2.29	2.17
V(N3) | V(N3,Ag1)*	2.99	2.81	3.00	3.08	3.01	3.1
V(N4,C3a)	2.30	2.31	2.31	2.34	2.34	2.38
V(N4) | V(N4,Ag2)*	2.75	3.08	2.79	2.87	2.86	2.99
V(N8,N1)	1.61	1.7	1.58	1.67	1.54	1.61
V(N8)	0.56	0.46	0.63	0.52	0.70	0.63
V(N8)	0.56	0.46	0.63	0.52	0.70	0.63

* Represents the monosynaptic basin population of the isolated ligand and its population once complexed with Ag, becoming to a disynaptic basin.