

Supporting Information

Silver(I)-based Energetic Coordination Polymers: Synthesis, Structure and Energy Performance

Xiaoni Qu, Sheng Zhang, Qi Yang, Zhiyong Su, Qing Wei,* Gang Xie, Sanping Chen*

^a Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi'an 710069, China.

Table of Contents:

Table S1. Selected bond lengths (Å) and bond angles (°) for **1**.

Table S2. Selected bond lengths (Å) and bond angles (°) for **2**.

Figure S1. XRPD curves for compounds **1** and **1a**.

Figure S2. XRPD curves for compounds **2** and **2a**.

Figure S3. The π - π overlap interactions between triazole rings in the adjacent layers in **1(a)** and **2(b)**.

Figure S4. The experimental luminescence decay of the free Hatz ligand monitored at excitation/emission 340/503 nm.

Figure S5. The experimental luminescence decay of the compound **1** monitored at excitation/emission 340/497 nm.

Figure S6. The experimental luminescence decay of the free Hntz ligand monitored at excitation/emission 384/495 nm.

Figure S7. The experimental luminescence decay of the compound **2** monitored at excitation/emission 384/503 nm.

*Corresponding author

Prof. Sanping Chen

Tel.: +8602988302604

Fax: +8602988302604
E-mail: sanpingchen@126.com

Table S1. Selected bond lengths (\AA) and bond angles ($^\circ$) for **1**.

| | | | |
|---------------------|------------|-------------------|------------|
| Ag(1)-N(3)#1 | 2.212(3) | N(2)-Ag(1)-N(1)#2 | 108.07(13) |
| Ag(1)-N(2) | 2.267(4) | C(2)-N(2)-Ag(1) | 127.4(3) |
| Ag(1)-N(1)#2 | 2.269(4) | N(1)-N(2)-Ag(1) | 126.3(3) |
| N(1)-Ag(1)#2 | 2.269(4) | C(1)-N(1)-Ag(1)#2 | 127.0(3) |
| N(3)-Ag(1)#3 | 2.212(3) | N(2)-N(1)-Ag(1)#2 | 123.3(3) |
| N(3)#1-Ag(1)-N(2) | 125.06(13) | C(1)-N(3)-Ag(1)#3 | 126.0(3) |
| N(3)#1-Ag(1)-N(1)#2 | 126.86(13) | C(2)-N(3)-Ag(1)#3 | 127.7(3) |

Symmetry transformations used to generate equivalent atoms:

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

Table S2. Selected bond lengths (\AA) and bond angles ($^\circ$) for **2**.

| | | | |
|-------------------|----------|---------------------|------------|
| N(4)-Ag(1)#1 | 2.258(3) | C(4)-N(3)-Ag(1)#2 | 129.6(2) |
| N(3)-Ag(1)#2 | 2.261(3) | C(3)-N(3)-Ag(1)#2 | 129.3(2) |
| Ag(1)-N(4)#1 | 2.258(3) | N(4)#1-Ag(1)-N(3)#3 | 124.81(10) |
| Ag(1)-N(3)#3 | 2.261(3) | N(4)#1-Ag(1)-N(2) | 106.86(9) |
| Ag(1)-N(2) | 2.307(3) | N(3)#3-Ag(1)-N(2) | 126.87(10) |
| C(3)-N(4)-Ag(1)#1 | 126.9(2) | C(4)-N(2)-Ag(1) | 128.4(2) |
| N(2)-N(4)-Ag(1)#1 | 127.3(2) | N(4)-N(2)-Ag(1) | 123.9(2) |

Symmetry transformations used to generate equivalent atoms:

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

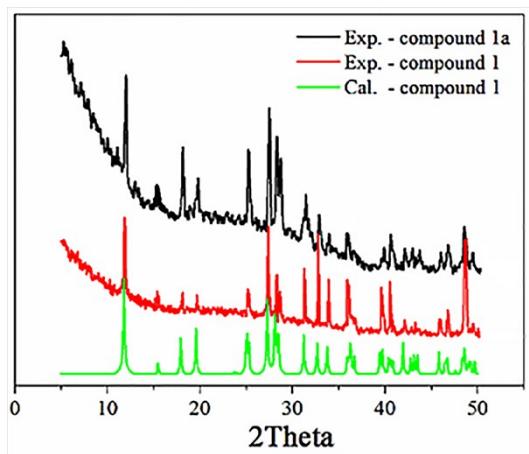


Figure S1. XRPD curves for compounds **1** and **1a**.

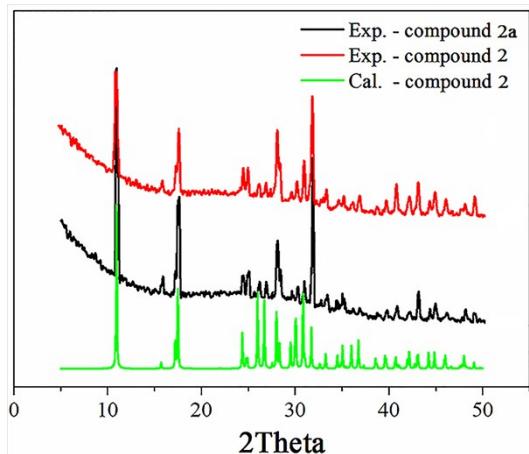


Figure S2. XRPD curves for compounds **2** and **2a**.

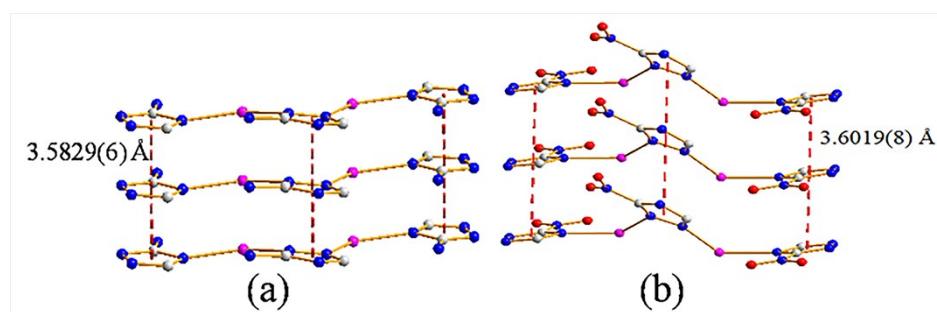


Figure S3. The π - π overlap interactions between triazole rings in the adjacent layers in **1** (a) and **2** (b).

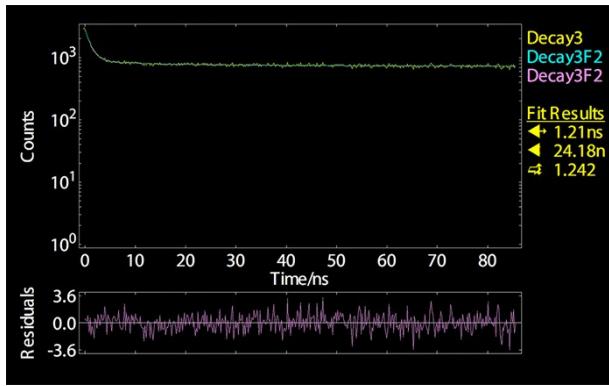


Figure S4. The experimental luminescence decay of the free Hatz ligand monitored at excitation/emission 340/503 nm.

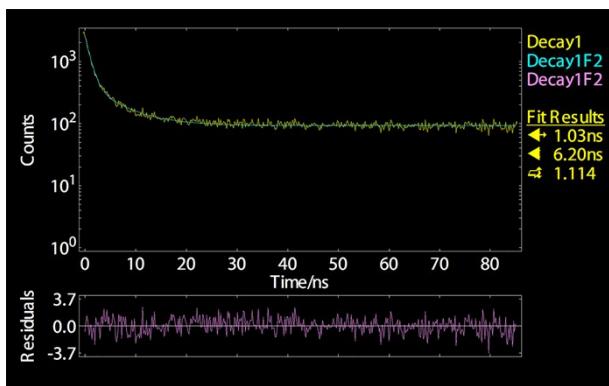


Figure S5. The experimental luminescence decay of the compound **1** monitored at excitation/emission 340/497 nm.

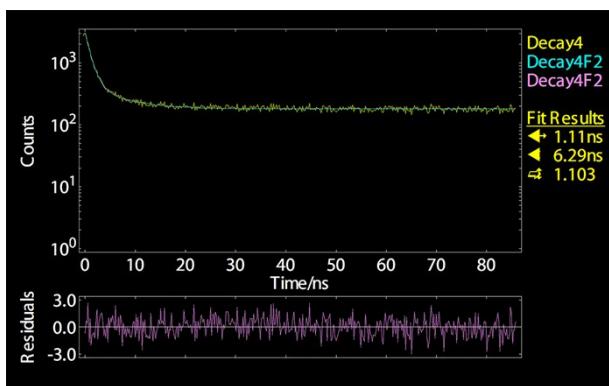


Figure S6. The experimental luminescence decay of the free Hntz ligand monitored at excitation/emission 384/495 nm.

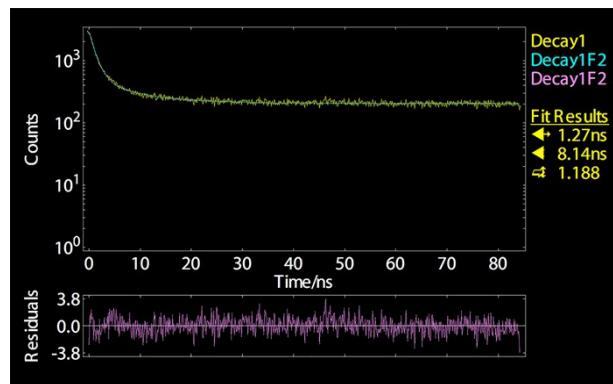


Figure S7. The experimental luminescence decay of the compound **2** monitored at excitation/emission 384/503 nm.