Supporting Information

A One-dimensional Infinite Silver Alkynyl Assembly $[Ag_8(C{\equiv}C^tBu)_5(CF_3COO)_3(CH_3CN)]_n$: Synthesis, Crystal Structure and Properties

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1. Synthetic procedures

General comments: In this paper, all reagents and solvents for synthesis were obtained from commercial sources and used without further purification, such as 3, 3-Dimethyl-1-butyne (Aladdin, >95%). All other reagents were of analytical grade and used as received. $[AgC{\equiv}C^tBu]_n$ was synthesized according to the literature.[1]

$[Ag_8(C{\equiv}C^tBu)_5(CF_3COO)_3(CH_3CN)]_n$ (1)

$[AgC{\equiv}C^tBu]_n$ (0.0566 g, 0.2994mmol) and CF_3COOAg (0.0660 g, 0.2987 mmol) were dissolved in 5 mL acetonitrile under stirring at room temperature. Then the mixture was transferred into a Teflon-lined stainless autoclave and kept at 70 ºC for 24 h. After cooling to room temperature, the yellow suspension was filtered and the filtrate slowly evaporated at room temperature in an Erlenmeyer flask. Two days later, we have successfully achieved the colorless block crystal **1**. Yield: ca. 53% (based on Ag). Elemental analysis calcd (%) for $C_{38}H_{48}Ag_8F_9NO_6$: C, 27.68; H, 2.93; N, 0.85; found: C, 27.70; H, 2.91; N, 0.86.

2. Crystallographic studies

Single-crystal X-ray diffraction data for **1** were recorded on a Bruker D8 QUEST with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) at 296(2) K. Absorption corrections were applied using multi-scan technique and performed by using the SADABS program. The crystal structure was solved by means of direct methods and refined by employing full-matrix least squares on F^2 (*SHELXL*-2017).[2] CCDC-1978916 (**1**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/ data_request/cif for **1**. Crystal data and structure refinements for compound **1** are listed in Table S1.

Table S1. Crystal data, data collection and structure refinement details for compound **1**

Compound	**1**
Formula	$C_{38}H_{48}Ag_8F_9N_1O_6$
Formula weight	1648.73
Crystal system	Triclinic
Space group	P -1
a (Å)	12.8132(6)
b (Å)	14.3594(7)
c (Å)	15.7145(7)
α (°)	101.9000(10)
β (°)	92.7640(10)
γ (°)	115.5780(10)
V (Å^3)	2520.9(2)
Z	2
D_c/g cm^{-3}	2.172

μ/mm^{-1}	3.112
F(000)	1576
Reflection collected	21064
Unique reflections	8831
Parameters	682
R_{int}	0.0195
GOF	1.024
$R_1{}^a$ [I>2σ(I)]	0.0264
$wR_2{}^b$(all data)	0.0654

$^aR_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; $^bwR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

Table S2. Selected bond lengths (Å) for compound **1**

Ag(1)-O(1)	2.309(4)		Ag(4)-O(5)	2.517(3)
Ag(1)-C(1)	2.428(4)		Ag(5)-O(4)	2.300(3)
Ag(1)-O(5)#1	2.443(3)		Ag(5)-C(13)	2.353(4)
Ag(1)-C(1)#1	2.447(4)		Ag(5)-C(19)	2.354(4)
Ag(2)-C(1)	2.165(4)		Ag(6)-O(6)	2.288(3)
Ag(2)-C(7)	2.237(4)		Ag(6)-C(25)	2.368(4)
Ag(2)-O(2)	2.348(3)		Ag(6)-C(19)#2	2.380(4)
Ag(3)-O(3')	2.32(4)		Ag(6)-C(13)	2.532(4)
Ag(3)-C(1)	2.322(4)		Ag(7)-C(19)	2.072(4)
Ag(3)-C(13)	2.344(4)		Ag(7)-C(25)	2.098(4)
Ag(3)-O(3)	2.361(14)		Ag(8)-N(1)	2.239(5)
Ag(3)-C(2)	2.629(4)		Ag(8)-C(25)	2.317(4)
Ag(4)-C(7)	2.134(4)		Ag(8)-C(7)#2	2.408(4)
Ag(4)-C(13)	2.145(4)		Ag(8)-C(26)	2.578(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+2; #2 -x+1,-y+1,-z+1.

Table S3. All the Ag···Ag interactions (Å) for compound **1**

Ag(1)-Ag(1)#1	2.9232(6)		Ag(4)-Ag(7)#2	3.0353(4)
Ag(1)-Ag(2)	2.9859(4)		Ag(4)-Ag(5)	3.2747(5)
Ag(1)-Ag(2)#1	2.9917(5)		Ag(5)-Ag(7)	3.0000(5)
Ag(1)-Ag(3)#1	3.1730(5)		Ag(5)-Ag(7)#2	3.0292(5)
Ag(2)-Ag(4)	2.8746(4)		Ag(5)-Ag(6)#2	3.1526(5)
Ag(2)-Ag(3)	2.9946(5)		Ag(5)-Ag(8)#2	3.2117(5)
Ag(3)-Ag(4)	2.8285(5)		Ag(6)-Ag(7)	2.8706(4)
Ag(4)-Ag(6)	2.8949(4)		Ag(6)-Ag(7)#2	3.1297(5)
Ag(4)-Ag(8)#2	2.9849(5)		Ag(7)-Ag(8)	2.9998(5)

3. Physical Measurements

Elemental analyses (C, H, and N) were performed on a Perkin-Elmer 2400 CHN elemental analyzer. PXRD patterns were recorded on a Siemens D 5005 diffractometer with Cu-Kα (λ= 1.5418 Å) radiation in the range of 3-50 ºC. The FT-IR spectrum was recorded from KBr pellets in the range of 4000–400 cm^{-1} on a Mattson Alpha-Centauri spectrometer. TGA was performed on a Q600 analyzer heated from room temperature to 900 ºC under nitrogen gas with a heating rate of 10 ºC/min. The UV-Vis absorption spectroscopy and diffuse reflectivity were measured on an UV-3600 UV-VIS-NIR spectrophotometer. Luminescence was measured on an FLS920 Full-featured fluorescence spectrometer.

Photoelectrochemical measurements

The photoelectrochemical (PEC) measurements were evaluated using a typical three-electrode configuration on an electrochemical workstation (CHI 660E, CH Instruments). The compound **1** coated fluorine-doped tin oxide (FTO) glass, Pt plate and Ag/AgCl were used as working, counter and reference electrodes, respectively. A 300 W Xe lamp (Perfect Light solar simulator) equipped with an AM 1.5 filter was utilized as the light source, and a 0.2 M Na_2SO_4 aqueous solution was used as the electrolyte. The working electrodes were prepared as the following method: 10 mg of as-synthesized sample was dispersed into 1mL of ethanol under sonication for 30 min to get a colloidal dispersion. Subsequently, the suspension was evenly dropped onto the surface of FTO glass. After air-dried at room temperature, the uncoated part of the FTO glass was isolated with epoxy resin glue.

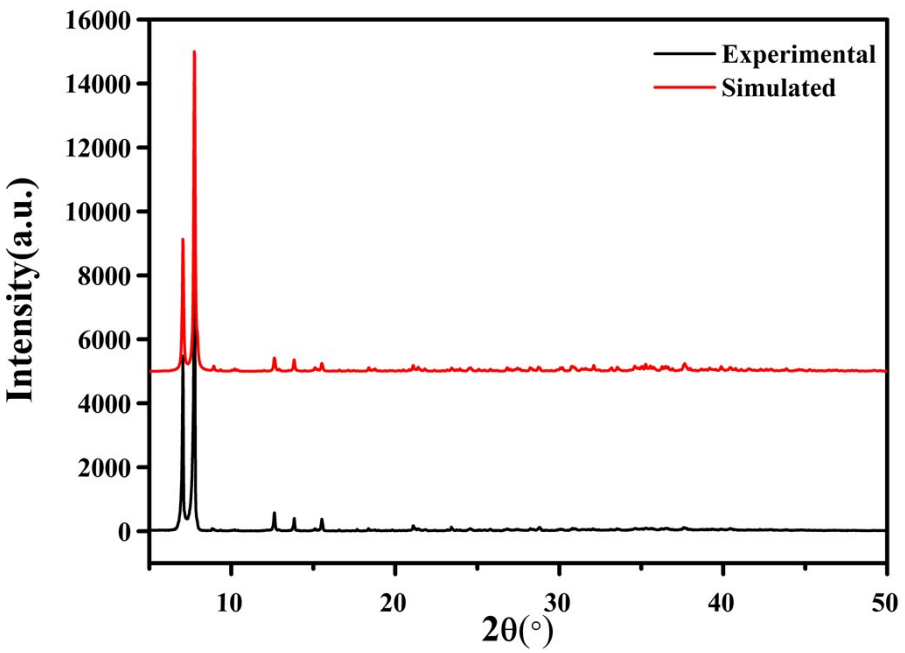

Figure S1. PXRDs of **1**.

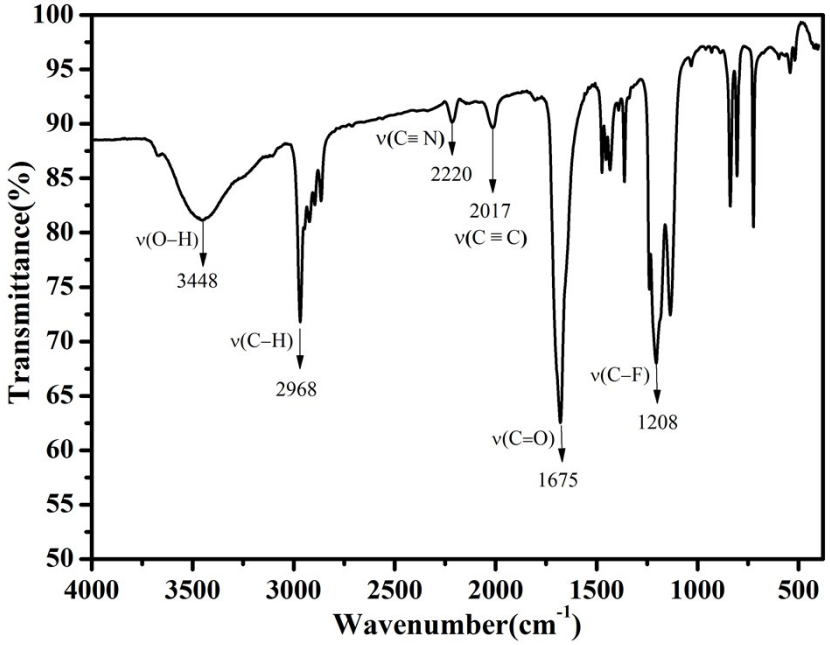

Figure S2. The IR spectrum of **1**

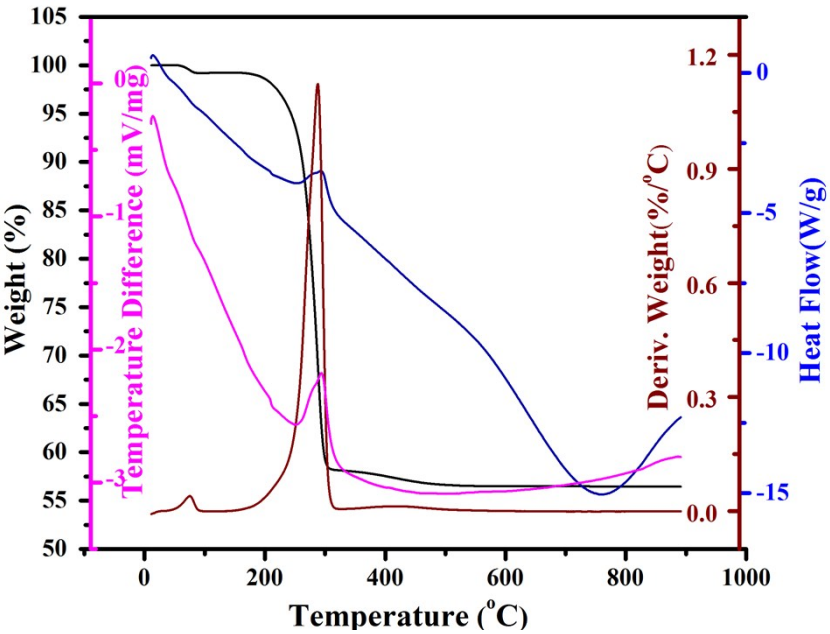

Figure S3. TGA/DSC curve of **1** (in N_2)

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Reference:

1 (a) Q.-M. Wang and T. C. W. Mak, *J. Am. Chem. Soc.*, 2000, **122**, 7608–7609; (b) M.-L. Chen, X.-F. Xu, Z.-X. Cao and Q.-M. Wang, *Inorg. Chem.*, 2008, **47**, 1877–1879.

2 G. M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3–8.