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Supporting Information

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Unprecedented Solution-Stable Silver(I) Ethynediyl Clusters

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Supporting information for:

Unprecedented Solution Stable Silver(I) Ethynediyl Clusters

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I. Physical measurements

X-ray experimental

II. Characterization

Figure S1. The ^1H NMR spectrum of complex **1** in CD_3OD .

Figure S2. The ^1H NMR spectrum of complex **1** in CD_3OD .

Figure S3. The ^1H NMR spectrum of complex **2** in CD_3OD .

Figure S4. The ^1H NMR spectrum of complex **2** in CD_3OD .

Figure S5. The molecular structure of **2**.

I. Physical measurements

(Trimethylsilyl)acetylene, 2,2'-Bipyridine (bpy), 1,10-Phenanthroline (phen) and all the solvents employed were commercially available and used as received. The C, H and N analyses were carried out with a Vario El III microanalyzer. The FT-IR spectra were recorded from KBr pellets in the range 4000-400 cm^{-1} with a Nicolet AVATAR FT-IR360 spectrometer. NMR data were recorded on a Bruker Avance II spectrometer (400MHz). Emission spectra were taken with HITACHI F7000 Spectrofluorometer. Raman spectroscopy was obtained using a LabRan-I Bilor Raman system with a 632.8 nm line from He-Ne laser.

X-ray experimental

Intensity data of compound **1** \cdot CH_3CN \cdot $0.5\text{CH}_3\text{OH}$ and **2** \cdot $2\text{CH}_2\text{Cl}_2$ were collected on a Oxford Gemini S Ultra system with Mo $\text{K}\alpha$ at 173 K and 123K, respectively. Data reductions were performed using CrysAlis RED program. The structure of **1** were solved by direct methods using SHELXS-97 and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms (except for the disordered methanol solvent molecule) using SHELXL-97. One trifluoroacetate anion is disordered over two set positions with 0.6 and 0.4 occupancy, respectively. For **2**, only silver atoms were refined by full-matrix least-squares on F^2 with anisotropic displacement parameters due to its poor crystal quality. Hydrogen atoms were calculated in ideal positions with isotropic displacement parameters set to $1.2 \times \text{U}_{\text{eq}}$ of the attached atom ($1.5 \times \text{U}_{\text{eq}}$ for methyl hydrogen atoms). No attempts were made to include hydrogen atoms of the disordered methanol solvent molecule in **1** and the water molecules in **2**.

II. Characterization

Ag7C2 (bpy) 5 (tfa) 5MeCN / CD3OD 090323

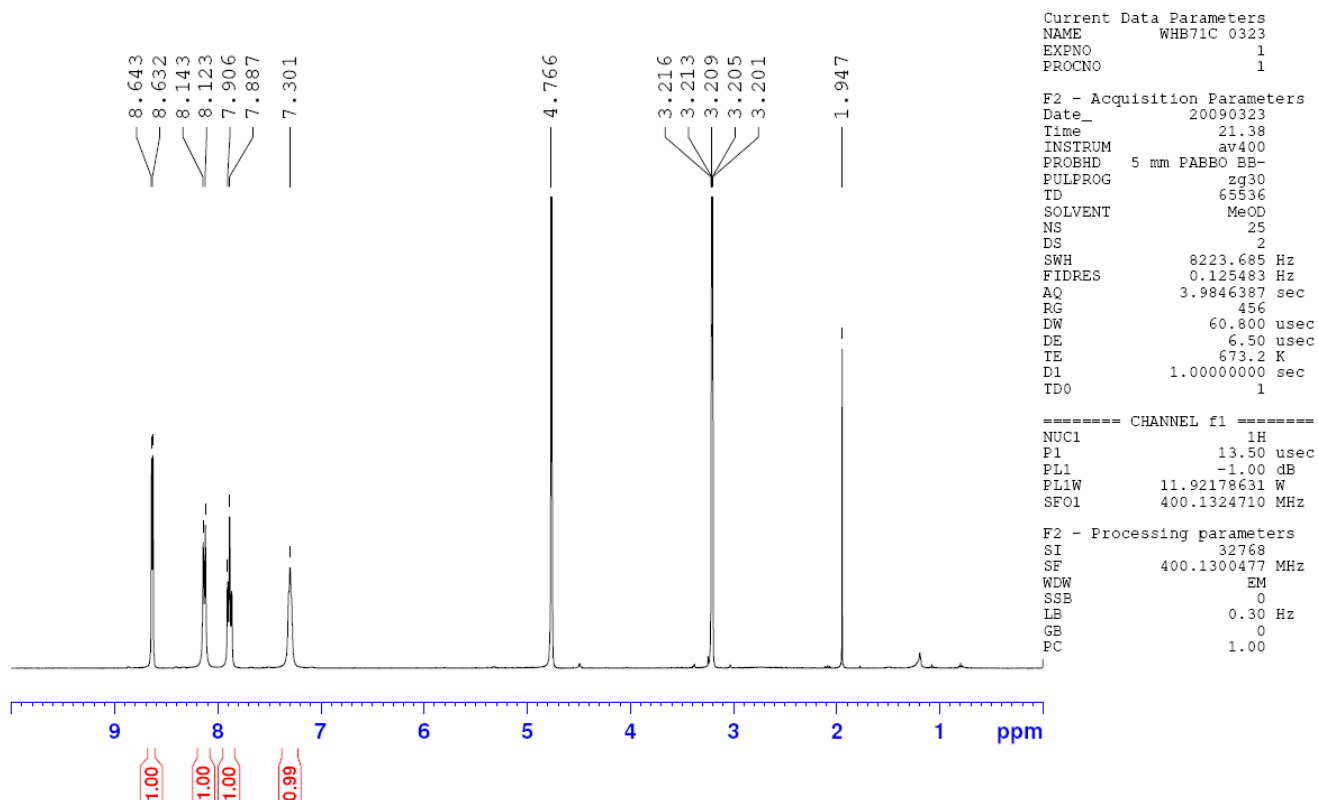


Figure S1. The ^1H NMR spectrum of complex **1** in CD_3OD .

Ag7C2 (bpy)5 (tfa)5 /CD3OD 090323



Current Data Parameters
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EXPNO 1
PROCNO 1

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Date_ 20090323
Time 21.38
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PULPROG zg30
TD 65536
SOLVENT MeOD
NS 25
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 456
DW 60.800 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1

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PL1 -1.00 dB
PL1W 11.92178631 W
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F2 - Processing parameters
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PC 1.00

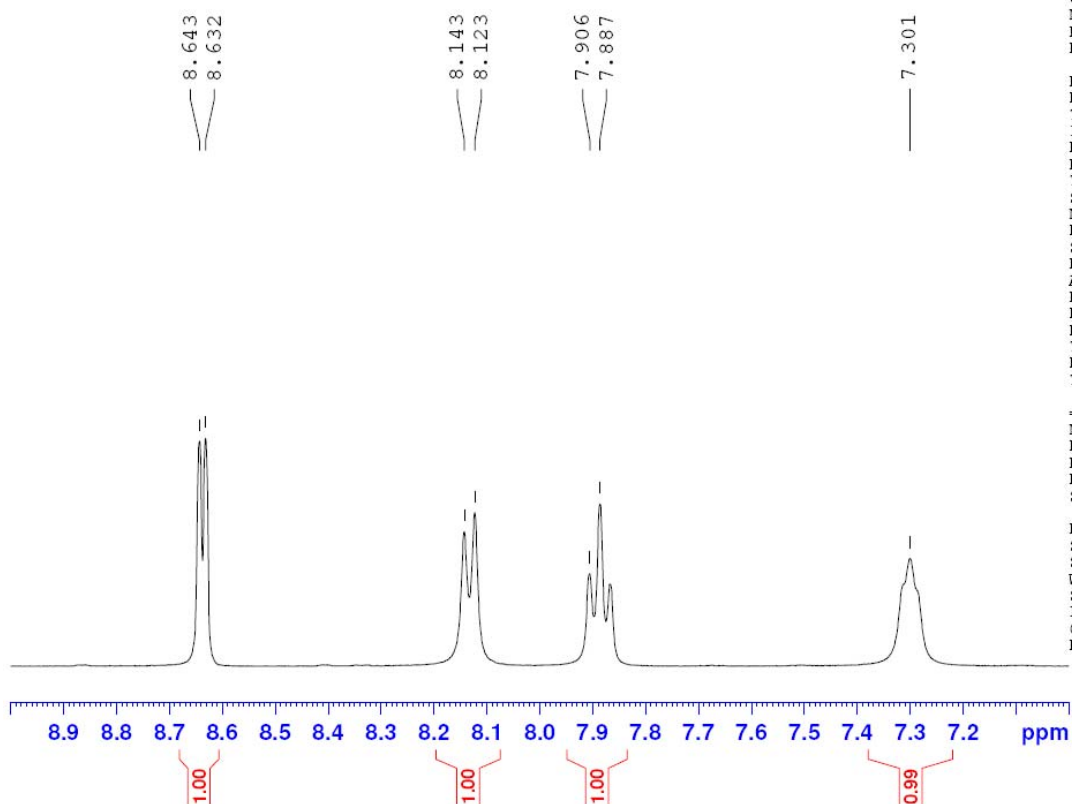


Figure S2. The ^1H NMR spectrum of complex **1** in CD_3OD .

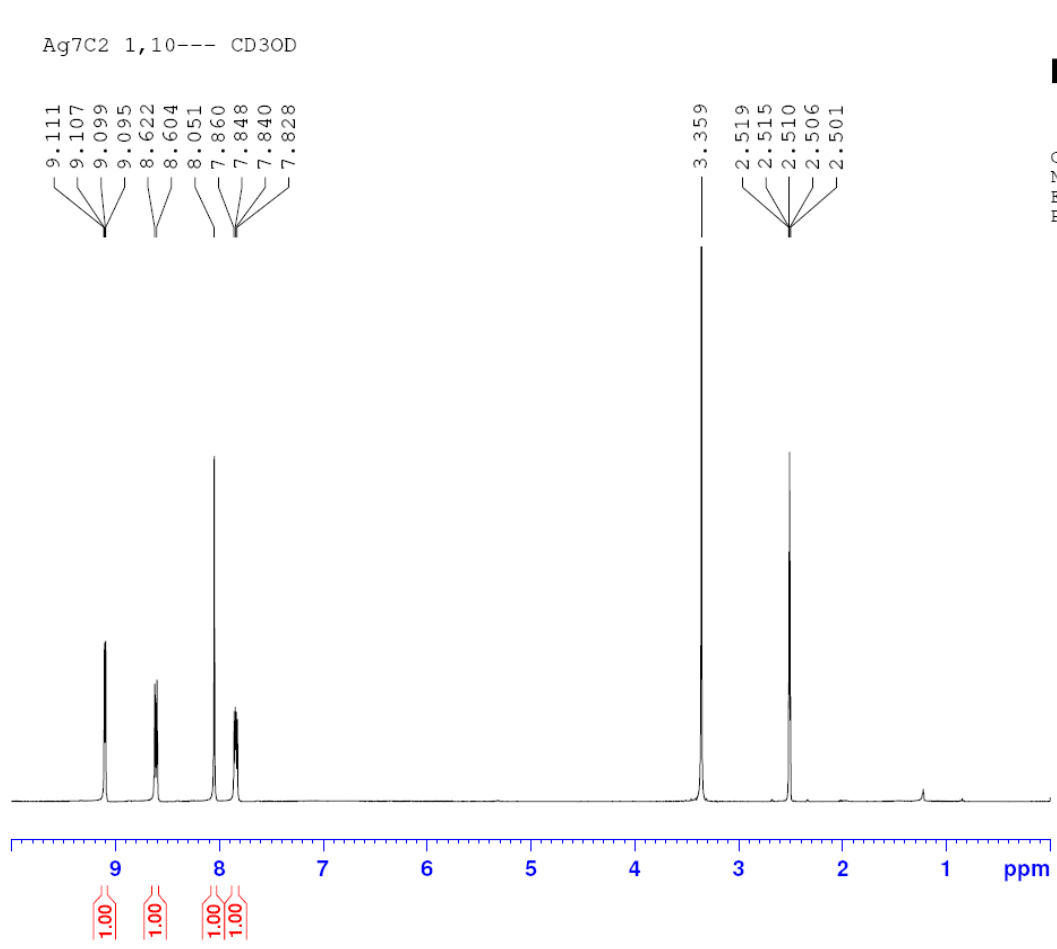


Figure S3. The ^1H NMR spectrum of complex **2** in CD_3OD .

Ag7C2 1,10--- CD3OD



Current Data Parameters
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EXPNO
PROCNO

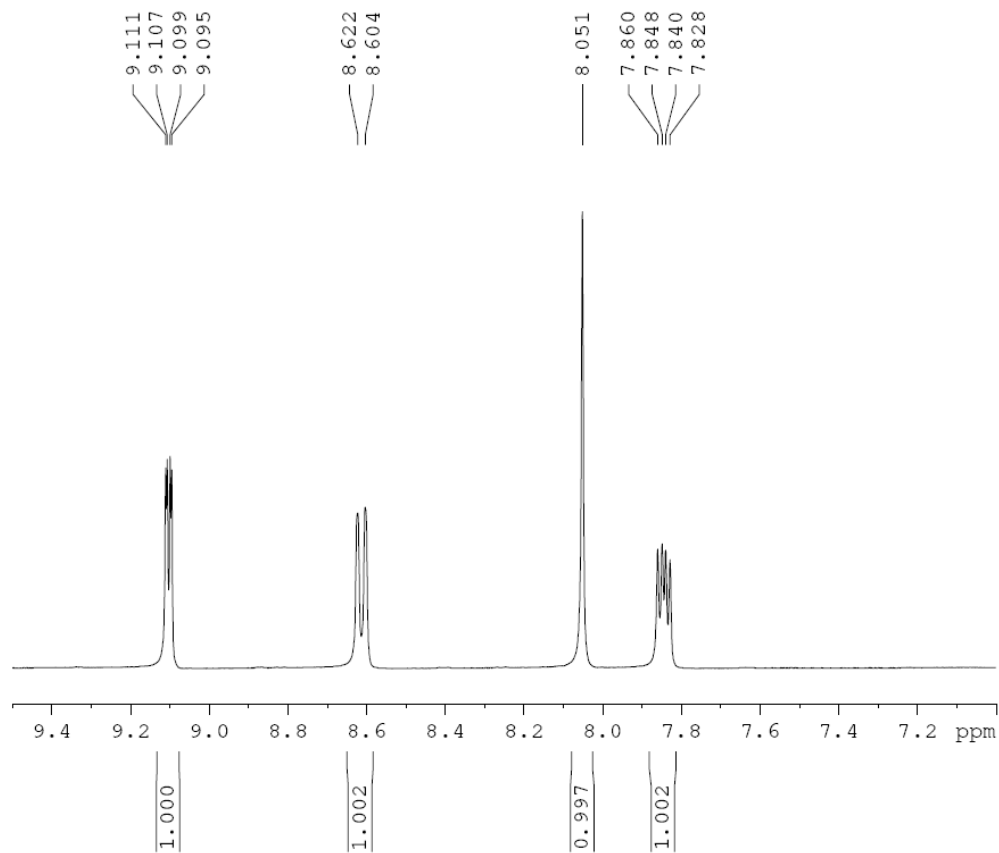


Figure S4. The ^1H NMR spectrum of complex **2** in CD_3OD .

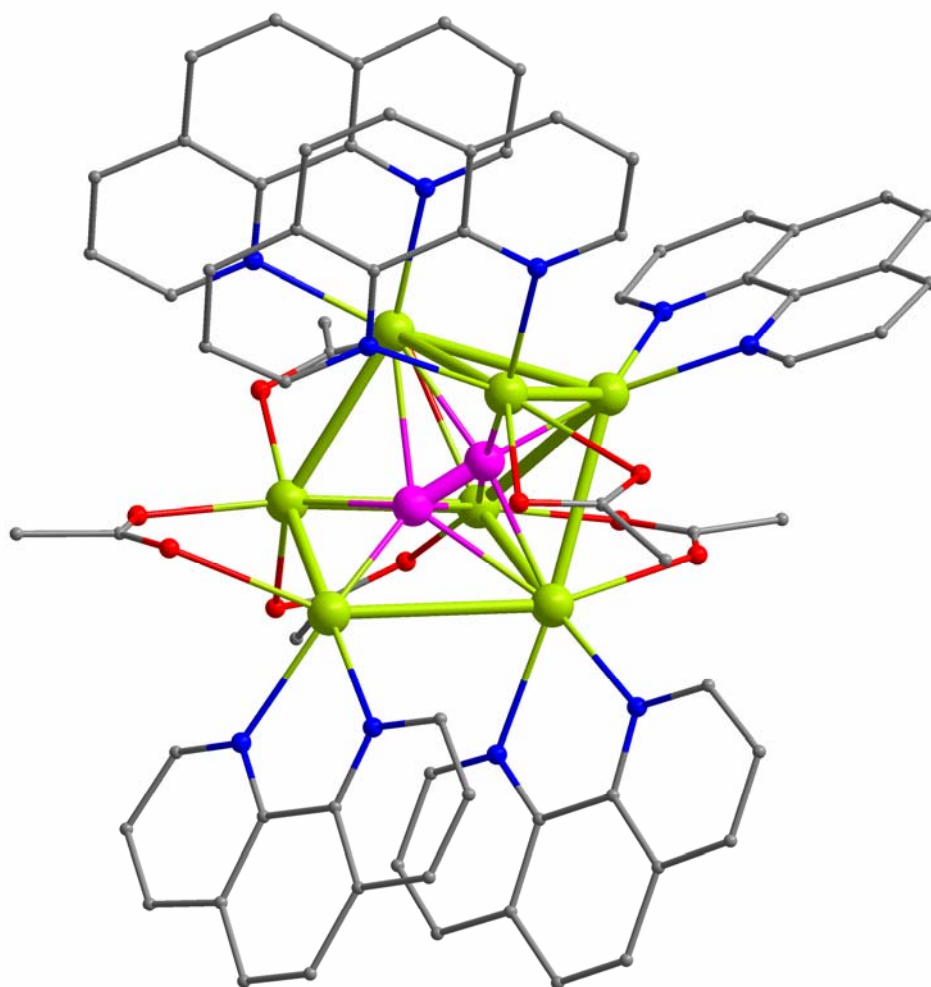


Figure S5. The molecular structure of **2**. Color legend: green, Ag; purple, C_2^{2-} ; red, O; blue, N; gray, C.