

Supplementary Information

Snowman-like silver alkynyl cluster consolidated by templating chloride and peripheral trifluoroacetates

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Materials and Methods. All reagents and solvents employed were commercially available and used as received without further purification. The C, H, and N microanalyses were carried out with a CE instruments EA 1110 elemental analyzer. 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). ESI-MS spectra were recorded on an ion trap mass spectrometer (Bruker, Esquire HCT).

X-ray experimental

Intensity data of compounds **1-3** were collected on a Oxford Gemini S Ultra system with Cu K α for **1** and **2**, Mo K α for **3**. Data collections were conducted at 173 K. Data reductions were performed using CrysAlis RED program. The structures 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 O31, O32, C31, C32, F31, F32, F33, O41, O42, C41, C42, F41, F42 in **1** and O71, O72, C71, C72, F71, F72, F73 in **3**) using SHELXL-97. Hydrogen atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2 \times U $_{eq}$ of the attached atom (1.5 \times U $_{eq}$ for methyl hydrogen atoms). Because a number of terminal C atoms of *tert*-butyl groups and terminal F atoms of CF $_3$ groups are not well resolved, thermal motion of the terminal C and F atoms are restrained by SIMU. DFIX restraints were also used for reasonable bond distances of *tert*-butyl and CF $_3$ groups. Totally 136 restraints have been applied in the structural refinement of **1**, and 78 for **2**, 487 for **3**.

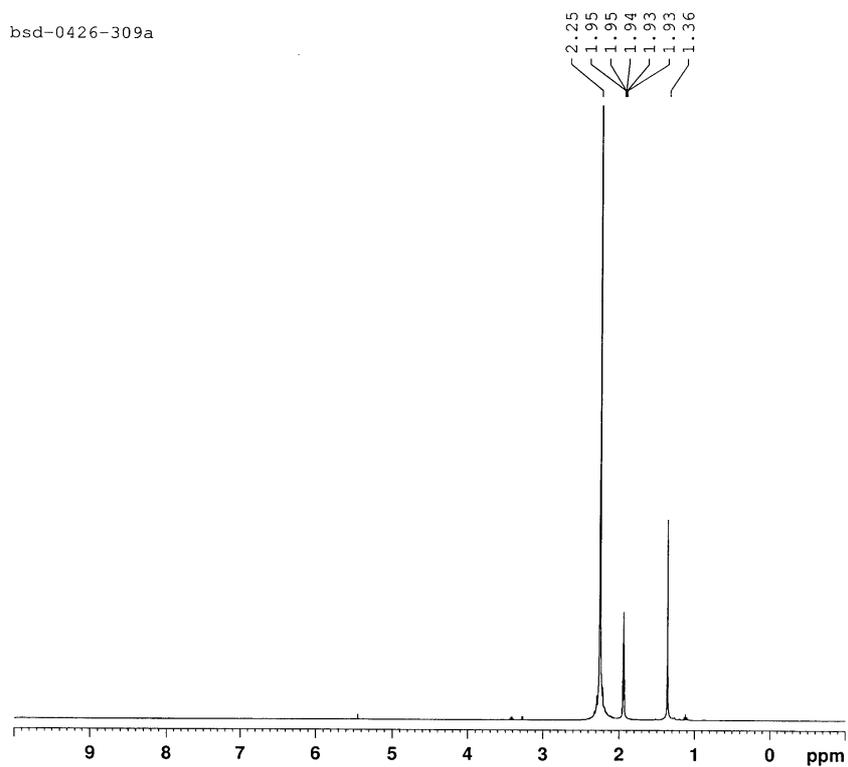


Figure S1. ^1H NMR spectrum of complex **1** at room temperature in CD_3CN . 2.25 (H_2O), 1.94 (solvent) and 1.36 ppm (CMe_3).

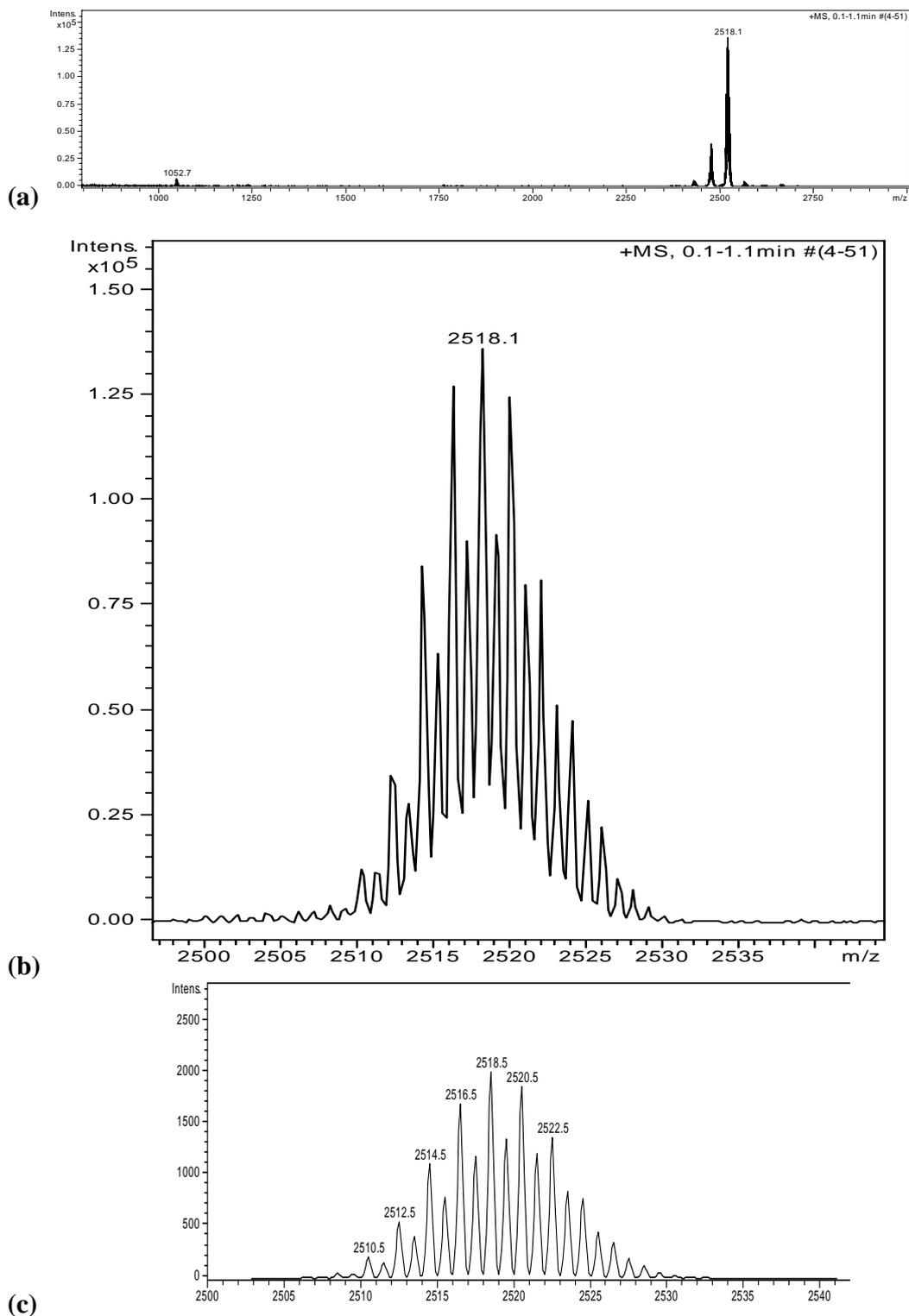


Figure S2. (a) ESI-MS spectra of complex **1** at room temperature in CH₃OH; (b) MS pattern observed at 2518.1; (c) Simulated ESI-MS pattern for [Ag₁₄(C≡CBu^t)₁₂Cl]⁺.