

Supplementary Material

Coordination Networks Constructed with the Supramolecular Synthon 4-Nitrophenyl-C≡C \supset Ag_n (n = 3, 4, 5)

Siegfried M. J. Wang, Liang Zhao and Thomas C. W. Mak*

*Department of Chemistry and Center of Novel Functional Molecules, The Chinese
University of Hong Kong, Shatin, New Territories, Hong Kong SAR, P. R. China.*

Fax: +852-26035057. E-mail: tcwmak@cuhk.edu.hk

Selected bond length information in regard to ethynide-silver coordination geometries in compound 3, 4, 6 and 10.

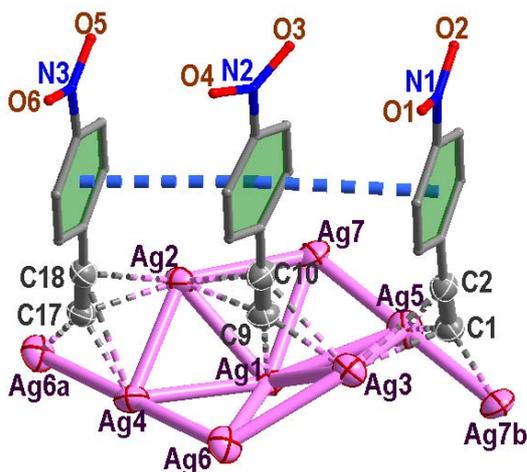


Fig. S1. Selected bond lengths information for compound 3 [Å]: C1≡C2 1.216(7), C9≡C10 1.199(7), C17≡C18 1.216(7), C1–Ag7b 2.086(5), C1–Ag3 2.425(5), C1–Ag5 2.172(5), C2–Ag3 2.734(5), C2–Ag5 3.045(5), C9–Ag1 2.114(5), C9–Ag2 2.433(5), C9–Ag3 2.378(5), C10–Ag2 2.906(5), C10–Ag3 2.818(5), C17–Ag6a 2.081(5), C17–Ag2 2.429(5), C17–Ag4 2.165(5), C18–Ag2 2.753(5), C18–Ag4 3.207(5), Ag7b⋯Ag5 2.841(1), Ag6a⋯Ag4 2.839(1), Ag1⋯Ag2 2.910(1), Ag1⋯Ag3 2.937(1), Ag1⋯Ag4 3.160(1), Ag1⋯Ag6 3.269(1), Ag1⋯Ag7 3.257(1), Ag2⋯Ag4 2.973(1), Ag2⋯Ag7 3.256(1), Ag3⋯Ag5 2.944(1), Ag3⋯Ag6 3.183(1), Ag4⋯Ag6 2.839(1), Ag5⋯Ag7 2.841(1), Symmetry code: a 1–x, 2–y, 2–z, b 2–x, 2–y, 2–z.

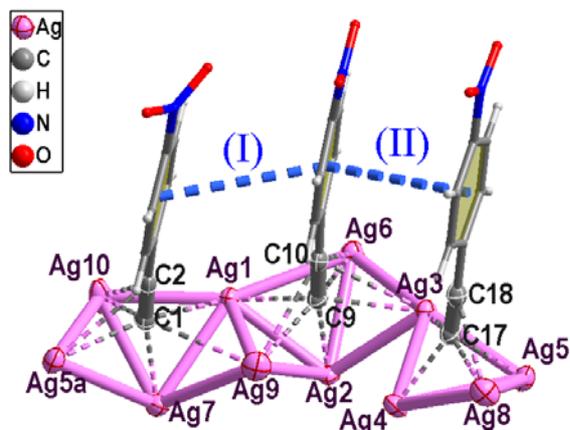


Fig. S2. Selected bond lengths information for compound **4** [Å]: C1≡C2 1.219(6), C9≡C10 1.223(6), C17≡C18 1.215(6), C1–Ag1 2.477(4), C1–Ag7 2.132(4), C1–Ag9 2.928(4), C1–Ag10 2.180(4), C1–Ag5a 2.432(4), C2–Ag10 2.973(4), C2–Ag5a 2.761(4), C9–Ag1 2.370(4), C9–Ag2 2.148(4), C9–Ag3 2.487(4), C9–Ag6 2.409(4), C9–Ag9 2.461(4), C10–Ag3 2.798(4), C10–Ag9 3.000(4), C17–Ag3 2.378(4), C17–Ag4 2.150(4), C17–Ag5 2.271(4), C17–Ag8 2.422(4), C18–Ag8 2.539(4), Ag1⋯Ag2 2.839(1), Ag1⋯Ag6 3.075(1), Ag1⋯Ag7 3.026(1), Ag1⋯Ag9 3.037(1), Ag1⋯Ag10 2.947(1), Ag2⋯Ag3 2.977(1), Ag2⋯Ag6 2.952(1), Ag2⋯Ag9 2.981(1), Ag3⋯Ag4 2.859(1), Ag3⋯Ag5 2.932(1), Ag3⋯Ag6 3.067(1), Ag4⋯Ag5 3.143(1), Ag4⋯Ag8 3.043(1), Ag5⋯Ag8 3.123(1), Ag7⋯Ag9 3.010(1), Ag7⋯Ag10 3.022(1), Ag7⋯Ag5a 3.011(1), Ag10⋯Ag5a 3.244(1). Symmetry code: $a\ x-1, y, z$.

4AgL · 4AgC₃F₇COO · 3CH₃CN (6)

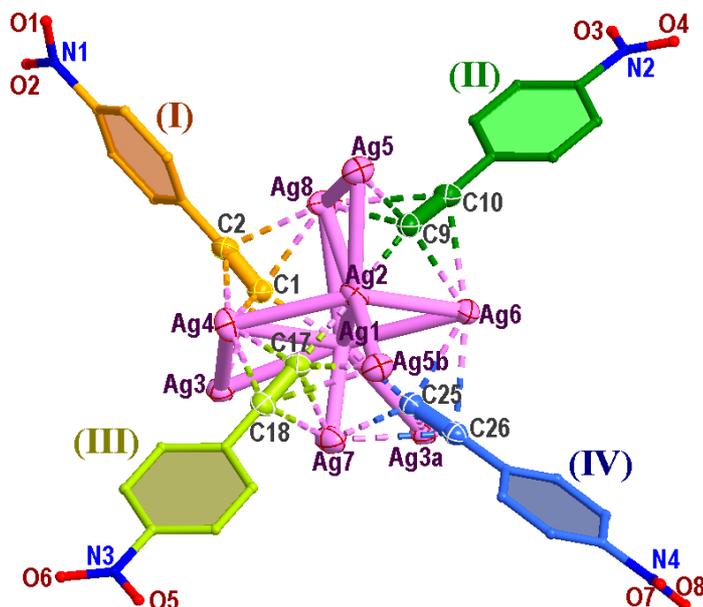
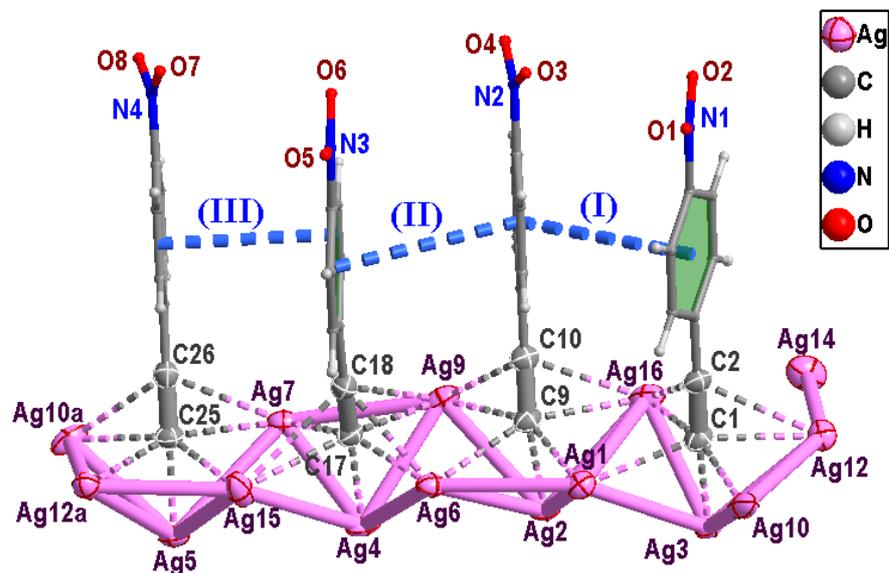
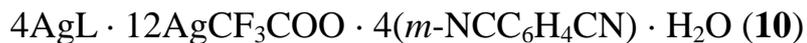
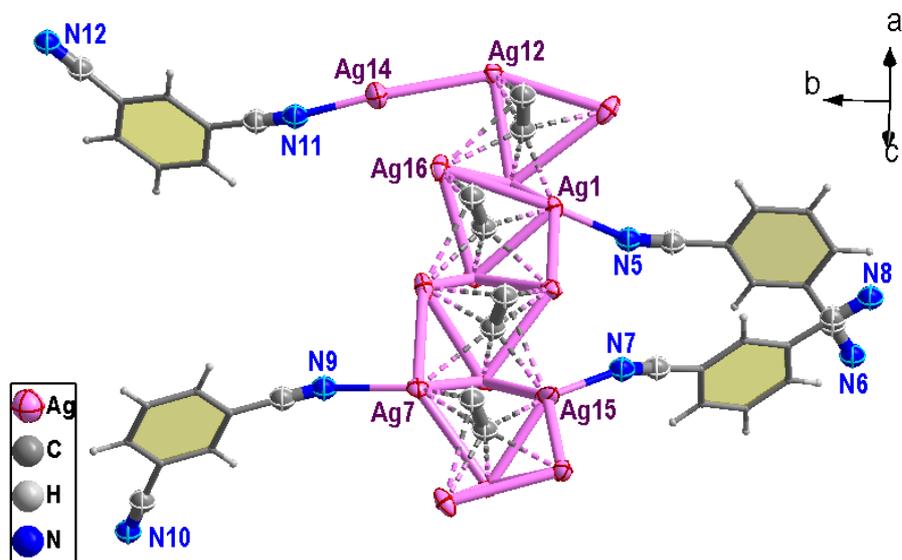


Fig. S3. Selected bond lengths information for compound **6** [Å]: C1≡C2 1.216(5), C9≡C10 1.223(5), C17≡C18 1.223(5), C17≡C18 1.222(5), C1–Ag1 2.122(4), C1–Ag3 2.437(3), C1–Ag4 2.430(3), C1–Ag8 2.507(4), C2–Ag4 2.950(3), C2–Ag8 2.598(4), C9–Ag2 2.114(4), C9–Ag5 2.387(4), C9–Ag6 2.389(4), C9–Ag8 2.348(4), C10–Ag6 2.582(4), C10–Ag8 2.782(4), C17–Ag2 2.104(4), C17–Ag4 2.389(4), C17–Ag5b 2.437(4), C17–Ag7 2.394(4), C18–Ag4 2.839(4), C18–Ag5b 2.874(4), C18–Ag7 2.668(4), C25–Ag1 2.135(4), C25–Ag6 2.410(4), C25–Ag7 2.345(4), C25–Ag3a 2.365(4), C26–Ag6 2.670(4), C26–Ag7 2.847(4), C26–Ag3a 2.807(4), Ag1⋯Ag2 3.093(1), Ag1⋯Ag3 2.874(1), Ag1⋯Ag4 3.202(1), Ag1⋯Ag6 3.045(1), Ag1⋯Ag7 2.951(1), Ag1⋯Ag8 3.136(1), Ag1⋯Ag3a 3.068(1), Ag2⋯Ag4 2.954(1), Ag2⋯Ag5 2.856(1), Ag2⋯Ag6 2.950(1), Ag2⋯Ag8 3.068(1), Ag2⋯Ag5b 2.954(1), Ag3⋯Ag4 2.922(1), Ag5⋯Ag8 3.285(1). Symmetry code: a $-x, -y, 2-z$; b $1-x, -y, 2-z$.



(a)



(b)

Fig. S4. (a) Silver-ethynide coordination environment in compound **10**. Selected bond lengths information for compound **10** [Å]: C1≡C2 1.223(9), C9≡C10 1.231(9), C17≡C18 1.211(9), C25≡C26 1.225(9), C1–Ag1 2.494(6), C1–Ag3 2.096(7), C1–Ag10 2.592(7), C1–Ag12 2.453(6), C1–Ag16 2.561(7), C2–Ag12, C2–Ag16, C9–Ag1 2.356(6), C9–Ag2 2.814(6), C9–Ag6 2.823(7), C9–Ag9 2.552(6), C9–Ag16 2.468(6), C10–Ag9 2.743(7),

C10–Ag16 2.683(6), C17–Ag4 2.111(7), C17–Ag6 2.748(6), C17–Ag7 2.659(7),
C17–Ag9 2.382(7), C17–Ag15 2.529(7), C18–Ag6 2.732(6), C18–Ag9 2.884(6),
C18–Ag15 2.898(7), C25–Ag5 2.122(7), C25–Ag7 2.679(6), C25–Ag15 2.352(6),
C25–Ag10a 2.493(6), C25–Ag12a 2.427(7), C26–Ag7 2.941(6), C26–Ag10a 2.843(7),
Ag1…Ag2 2.853(1), Ag1…Ag3 2.896(1), Ag1…Ag6 2.987(1), Ag1…Ag16 3.162(1),
Ag2…Ag6 3.108(1), Ag2…Ag9 3.115(1), Ag2…Ag16 3.032(1), Ag3…Ag10 3.228(1),
Ag3…Ag12 2.971(1), Ag3…Ag16 3.058(1), Ag4…Ag6 3.028(1), Ag4…Ag7 2.880(1),
Ag4…Ag9 2.972(1), Ag4…Ag15 3.066(1), Ag5…Ag7 3.208(1), Ag5…Ag15 2.818(1),
Ag5…Ag10a 2.922(1), Ag5…Ag12a 3.009(1), Ag7…Ag9 3.264(1), Ag12…Ag14 3.175(1),
Ag15…Ag12a 3.003(1), Ag10a…Ag12a 3.204(1). Symmetry code: a x , $1.5-y$, $0.5+z$, b x ,
 $1.5-y$, $-0.5+z$. **(b)** Geometrical arrangement of the nitrile ligands.