Electronic Supplementary Information

Formation of N-heterocyclic diphosphine ligands from Ag(I)-assisted condensation reactions between bdppeda and formaldehyde and their binuclear silver(I) complexes

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Contents

Scheme S1. Possible mechanism for the formation of $[Ag_2(L_1)_2(\eta,\eta\text{-}\mu\text{-}ClO_4)_2](ClO_4)_2$ (**1**) from reactions of $[Ag(MeCN)_4]ClO_4$ with bdppeda and HCOOH.
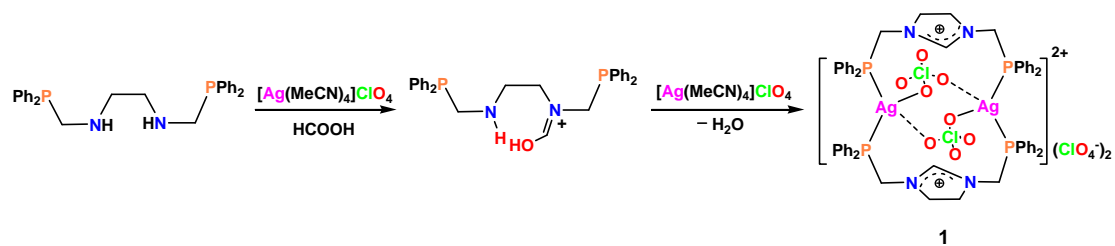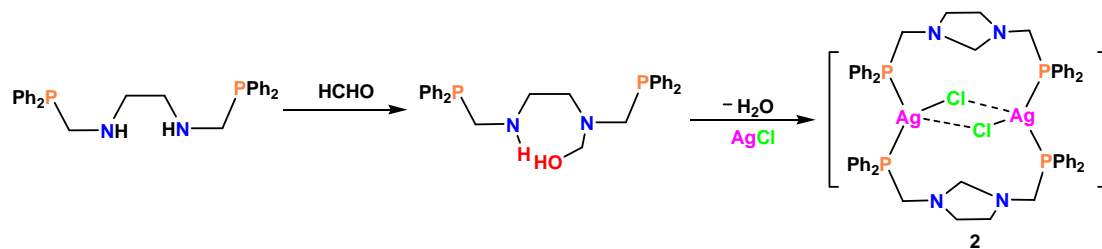

Scheme S2. Possible mechanism for the formation of $[Ag_2(L_2)_2(\mu\text{-}Cl)_2]$ (**2**) from reactions of AgCl with bdppeda and HCHO.

(a)

674   678   467   468   469

675.3   467.2
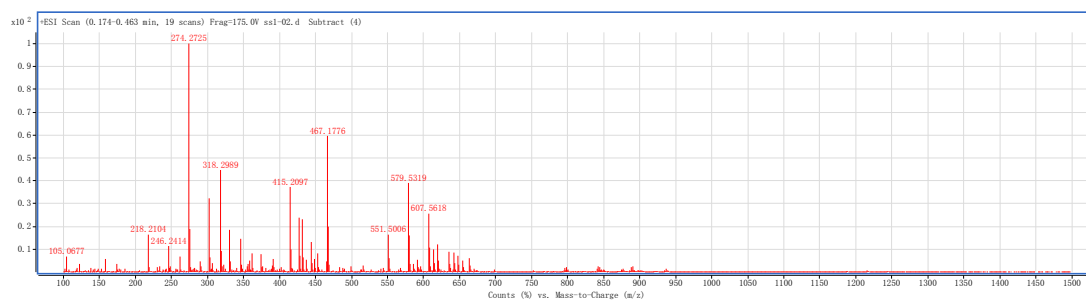
(b)   (c)

Figure S1. Positive-ion ESI MS of complex **1** in DMF. (a) The full data ranging from m/z = 100-1500; (b) tested (black) and simulated (gray) data at m/z = 675.3 for the parent dication $[Ag_2(L_1)_2(ClO_4)_2]^{2+}$; (c) tested (black) and simulated (gray) data at m/z = 467.2 for $[L_1]^+$ cation.

(a)

(b)   (c)   (d)

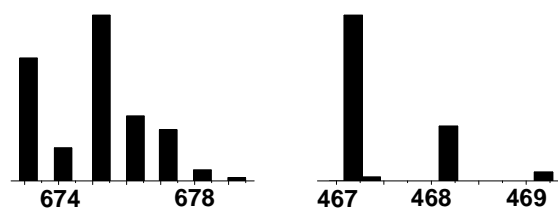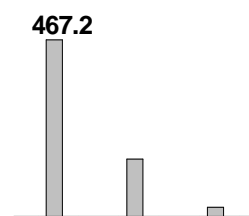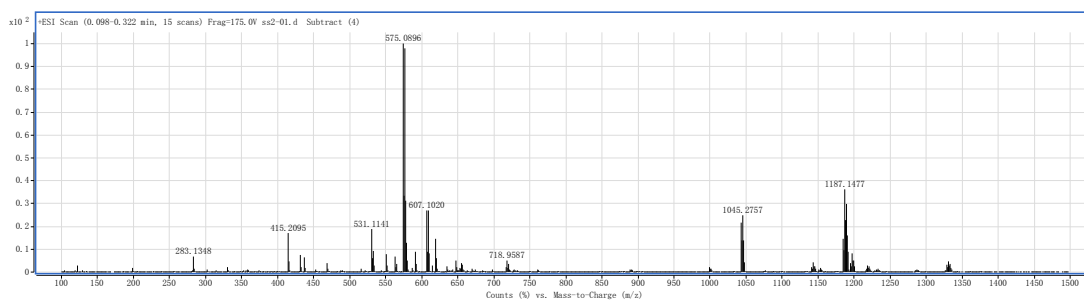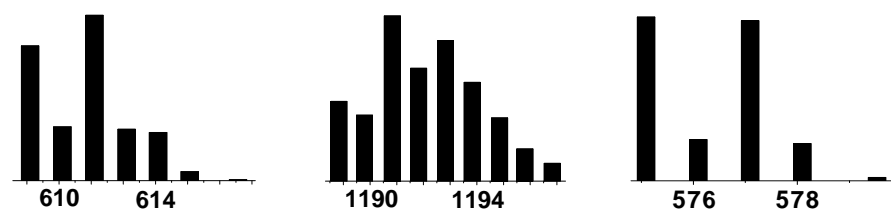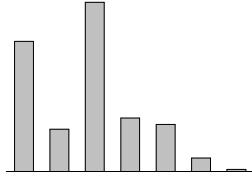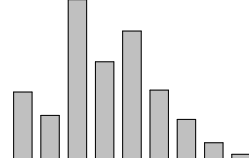**Figure S2**. Positive-ion ESI MS of complex **2** in DMF. (a) The full data ranging from $m/z =$ 100-1500; (b) The tested (black) and simulated (gray) data at $m/z = 609.1$ for the parent dication $[Ag_2(HL_2)_2Cl_2]^{2+}$; (c) The tested (black) and simulated (gray) data at $m/z = 1190.8$ for $[Ag_2(L_2)_2Cl]^+$ cation. (d) The tested (black) and simulated (gray) data at $m/z = 575.1$ for the $[Ag(L_2)]^+$ cation.

(a)
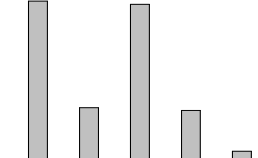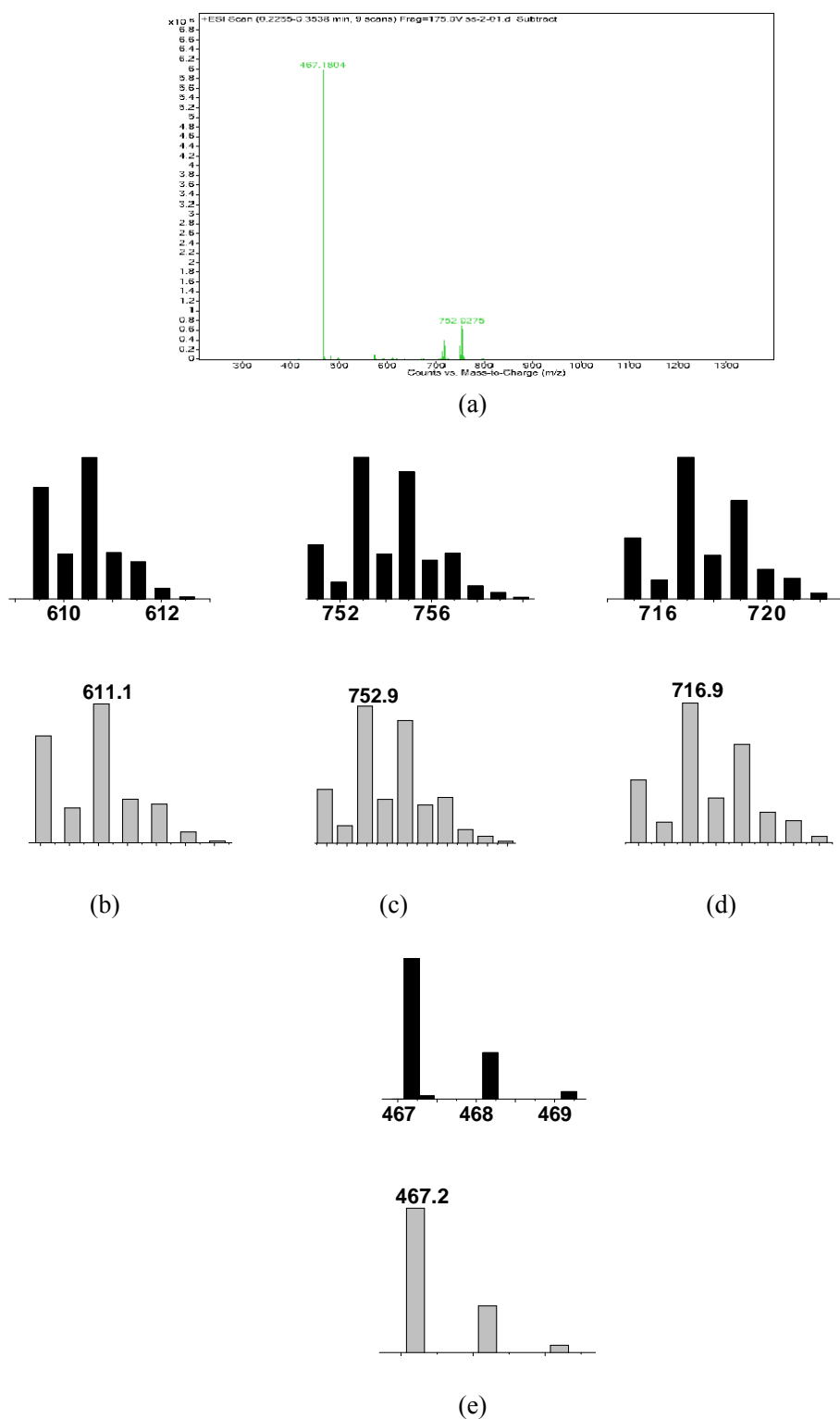

(b)   (c)   (d)


(e)

Figure S3. Positive-ion ESI MS of complex **3** in DMF. (a) The full data ranging from m/z = 100-1500; (b) The tested (black) and simulated (gray) data at m/z = 611.1 for the parent dication $[Ag_2(L_1)_2Cl_2]^{2+}$; (c) The tested (black) and simulated (gray) data at m/z = 752.9 for $[Ag_2(L_1)Cl_2]^+$ cation. (d) The tested (black) and simulated (gray) data at m/z = 716.9 for the $[Ag_2(L_1)Cl]^+$ cation. (e) tested (black) and simulated (gray) data at m/z = 467.2 for $[L_1]^+$ cation.

(a)

(b)

(c)
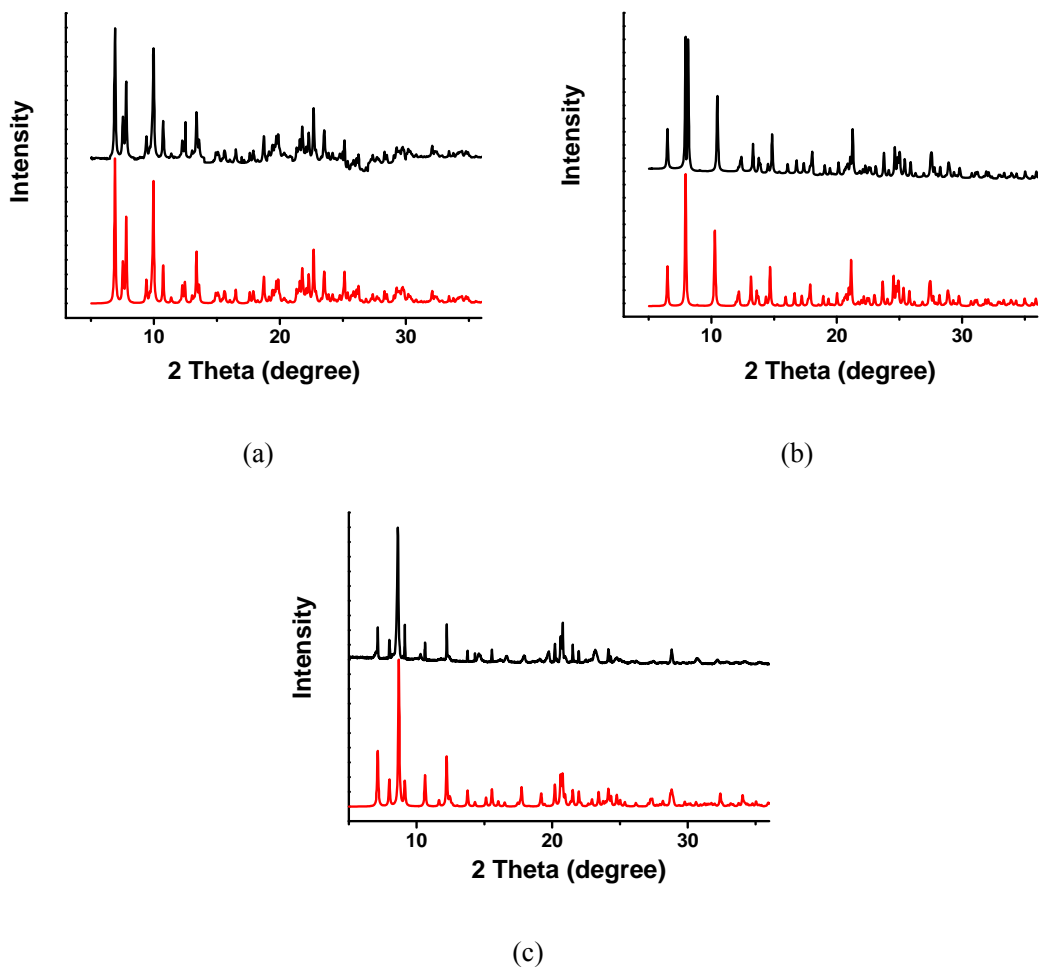
Figure S4. Experimental (black) and simulated (red) p-XRD patterns for **1** (a); **2**(b); **3**(c).