

Electronic Supplementary Information

Fascinating 3D energetic $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$: filling the ethylenediamine molecules into $[\text{Ag}(\text{N}_5)]_n$ framework

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1. Crystal data and structure refinement details of $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$, $[\text{Ag}(\text{N}_5)]_n$ and $[\text{Ag}_3(\text{N}_5)_4]_n \cdot n[\text{Ag}(\text{NH}_3)_2]$

Table S1. Crystal data and structure refinement details of $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$, $[\text{Ag}(\text{N}_5)]_n$ and $[\text{Ag}_3(\text{N}_5)_4]_n \cdot n[\text{Ag}(\text{NH}_3)_2]$

	$[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$	$[\text{Ag}_3(\text{N}_5)_4]_n \cdot n[\text{Ag}(\text{NH}_3)_2]$	$[\text{Ag}(\text{N}_5)]_n^1$
CCDC	2124736	1884910	1816845 ⁸
Empirical formula	CH_4AgN_6	$\text{Ag}_4\text{H}_6\text{N}_{22}$	$\text{Ag}_{16}\text{N}_{80}$
Formula weight	207.97	745.75	2846.72
Temperature	170.0 K	220 K	173 K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic	orthorhombic
Space group	$P2_1/c$	$P2_1/c$	Fddd
Unit cell dimensions	a=7.7903(2) Å b=8.9945(3) Å c=8.0367(2) Å $\alpha=90.00^\circ$ $\beta=116.1130(10)^\circ$ $\gamma=90.00^\circ$	a=9.0932(18) Å b=9.1069(17) Å c=9.8502(19) Å $\alpha=90.00^\circ$ $\beta=108.847(4)^\circ$ $\gamma=90.00^\circ$	a=11.904(2) Å b=15.240(3) Å c=17.282(3) Å $\alpha=90.00^\circ$ $\beta=90.00^\circ$ $\gamma=90.00^\circ$
Volume	505.65(3) Å ³	772.0(3) Å ³	3135.3(10) Å ³
Z	4	2	2
Density (calculated)	2.732 g·cm ⁻³	3.208 g·cm ⁻³	3.015 g·cm ⁻³
Absorption coefficient	3.870 mm ⁻¹	5.046 mm ⁻¹	4.958 mm ⁻¹
F(000)	396.0	696.0	2624.0
Crystal size	0.15 x 0.08 x 0.05 mm ³	0.12 x 0.06 x 0.03 mm ³	0.07 x 0.03 x 0.03 mm ³
Theta range for data collection	7.24 to 55.074 °	4.734 to 54.35°	4.94 to 49.988°
Index ranges	-8 ≤ h ≤ 10, -11 ≤ k ≤ 11, -10 ≤ l ≤ 9	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -12 ≤ l ≤ 12	—
Reflections collected	5749	6195	688
Independent reflections	1132 [R(int) = 0.0402, R(sigma)=0.0283]	1710 [R(int) = 0.0828, R(sigma)=0.0781]	688 [R(int) = 0, R(sigma)=0.1548]
Data / restraints / parameters	1132/0/73	1710/0/122	688/30/56
Goodness-of-fit on F ²	1.120	0.971	1.122
Final R indices [I > 2σ(I)]	R1=0.0188, wR ₂ =0.0412	R1=0.0415, wR ₂ =0.0654	R1=0.1063, wR ₂ =0.2723
R indices (all data)	R1=0.0216, wR ₂ =0.0430	R1=0.1100, wR ₂ =0.0840	R1=0.1816,

			wR ₂ =0.2892
Largest diff. peak and hole	0.311 and -0.308 e.Å ⁻³	0.95 and -0.86 e.Å ⁻³	1.64 and -1.77 e.Å ⁻³

2. Single-crystal X-ray diffraction analysis of [Ag₂(N₅)₂(EDA)]_n

Table S2. Crystal data, data collection, and refinement for [Ag₂(N₅)₂(EDA)]_n

CH ₄ AgN ₆	$F(000) = 396$
$M_r = 207.97$	$D_x = 2.732 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.7903 (2) \text{ \AA}$	Cell parameters from 4340 reflections
$b = 8.9945 (3) \text{ \AA}$	$\theta = 3.6\text{--}27.5^\circ$
$c = 8.0367 (2) \text{ \AA}$	$\mu = 3.87 \text{ mm}^{-1}$
$\beta = 116.113 (1)^\circ$	$T = 170 \text{ K}$
$V = 505.65 (3) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.15 \times 0.08 \times 0.05 \text{ mm}$
D8 VENTURE diffractometer	1051 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{\text{int}} = 0.040$
Absorption correction: multi-scan SADABS2016/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0810 before and 0.0542 after correction. The Ratio of minimum to maximum transmission is 0.8128. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.6^\circ$
$T_{\text{min}} = 0.754$, $T_{\text{max}} = 0.928$	$h = -8 \rightarrow 10$
5749 measured reflections	$k = -11 \rightarrow 11$
1132 independent reflections	$l = -10 \rightarrow 9$
Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.019$	H-atom parameters constrained
$wR(F^2) = 0.043$	$w = 1/[\sigma^2(F_o^2) + 0.4594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1132 reflections	$\Delta_{\text{max}} = 0.41 \text{ e \AA}^{-3}$
73 parameters	$\Delta_{\text{min}} = -0.38 \text{ e \AA}^{-3}$
0 restraints	

Table S3. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.68902 (3)	0.17021 (2)	0.58482 (2)	0.02381 (8)
N6	0.2354 (3)	0.4808 (2)	0.5357 (3)	0.0256 (4)
N5	0.3148 (3)	0.3813 (2)	0.4706 (3)	0.0227 (4)
N1	0.9749 (3)	0.1918 (2)	0.5794 (3)	0.0192 (4)
H1B	0.982000	0.282982	0.533611	0.023*
H1A	1.068748	0.186747	0.697592	0.023*
N4	0.3431 (3)	0.4920 (2)	0.7161 (3)	0.0230 (4)
N2	0.4705 (3)	0.3311 (2)	0.6109 (3)	0.0218 (4)
N3	0.4886 (3)	0.3997 (2)	0.7628 (3)	0.0230 (4)
C1	1.0105 (4)	0.0772 (3)	0.4673 (3)	0.0199 (5)
H1C	1.141233	0.089316	0.477773	0.024*
H1D	0.918657	0.089459	0.335407	0.024*

Table S4. Atomic displacement parameters (\AA^2) for $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.02235 (13)	0.02716 (13)	0.02388 (12)	0.00002 (7)	0.01197 (9)	-0.00276 (8)
N6	0.0219 (11)	0.0266 (11)	0.0245 (11)	0.0034 (9)	0.0069 (9)	0.0004 (9)
N5	0.0182 (10)	0.0270 (11)	0.0186 (10)	0.0003 (8)	0.0041 (8)	-0.0006 (9)
N1	0.0209 (11)	0.0167 (10)	0.0192 (10)	0.0000 (8)	0.0080 (8)	0.0005 (8)
N4	0.0235 (11)	0.0232 (11)	0.0220 (10)	0.0019 (8)	0.0098 (8)	-0.0022 (9)
N2	0.0243 (11)	0.0223 (11)	0.0192 (10)	0.0018 (8)	0.0100 (9)	-0.0006 (8)
N3	0.0233 (11)	0.0258 (11)	0.0177 (10)	0.0046 (9)	0.0068 (9)	0.0011 (9)
C1	0.0227 (13)	0.0187 (12)	0.0206 (12)	0.0004 (9)	0.0117 (10)	0.0018 (10)

Table S5. Geometric parameters (\AA , $^\circ$) for $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$

Ag1—N1	2.255 (2)	N1—H1A	0.9100
Ag1—N4 ⁱ	2.355 (2)	N1—C1	1.474 (3)
Ag1—N2	2.313 (2)	N4—N3	1.319 (3)
Ag1—N3 ⁱⁱ	2.444 (2)	N2—N3	1.319 (3)
N6—N5	1.319 (3)	C1—C1 ⁱⁱⁱ	1.520 (4)
N6—N4	1.321 (3)	C1—H1C	0.9900
N5—N2	1.320 (3)	C1—H1D	0.9900
N1—H1B	0.9100		

N1—Ag1—N4 ⁱ	118.24 (7)	N3—N4—Ag1 ^{iv}	124.75 (15)
N1—Ag1—N2	136.08 (7)	N3—N4—N6	108.39 (19)
N1—Ag1—N3 ⁱⁱ	100.25 (7)	N5—N2—Ag1	124.93 (16)
N4 ⁱ —Ag1—N3 ⁱⁱ	109.55 (7)	N3—N2—Ag1	126.40 (16)
N2—Ag1—N4 ⁱ	93.54 (7)	N3—N2—N5	108.34 (19)
N2—Ag1—N3 ⁱⁱ	95.97 (7)	N4—N3—Ag1 ^v	122.14 (15)
N5—N6—N4	107.76 (19)	N4—N3—N2	107.60 (19)
N6—N5—N2	107.9 (2)	N2—N3—Ag1 ^v	128.17 (15)
Ag1—N1—H1B	108.8	N1—C1—C1 ⁱⁱⁱ	110.5 (2)
Ag1—N1—H1A	108.8	N1—C1—H1C	109.6
H1B—N1—H1A	107.7	N1—C1—H1D	109.6
C1—N1—Ag1	113.89 (14)	C1 ⁱⁱⁱ —C1—H1C	109.6
C1—N1—H1B	108.8	C1 ⁱⁱⁱ —C1—H1D	109.6
C1—N1—H1A	108.8	H1C—C1—H1D	108.1
N6—N4—Ag1 ^{iv}	126.26 (15)		

Symmetry codes: (i) $-x+1, y-1/2, -z+3/2$; (ii) $x, -y+1/2, z-1/2$; (iii) $-x+2, -y, -z+1$; (iv) $-x+1, y+1/2, -z+3/2$; (v) $x, -y+1/2, z+1/2$.

Table S6. Hydrogen bonds (Å, °) for $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
N1—H1A \cdots N5	0.91	2.27	3.162(3)	166
N1—H1B \cdots N6	0.91	2.62	3.298(3)	132

3. Single-crystal X-ray diffraction analysis of $[\text{Ag}_3(\text{N}_5)_4]_n \cdot n[\text{Ag}(\text{NH}_3)_2]$

Table S7. Crystal data, data collection, and refinement for $[\text{Ag}_3(\text{N}_5)_4]_n \cdot n[\text{Ag}(\text{NH}_3)_2]$

$0.5(\text{Ag}_6\text{N}_{40}) \cdot \text{AgH}_6\text{N}_2$	$F(000) = 696$
$M_r = 745.75$	$D_x = 3.208 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 9.0932 (18) \text{ \AA}$	Cell parameters from 2704 reflections
$b = 9.1069 (17) \text{ \AA}$	$\theta = 2.4\text{--}22.3^\circ$
$c = 9.8502 (19) \text{ \AA}$	$\mu = 5.05 \text{ mm}^{-1}$
$\beta = 108.847 (4)^\circ$	$T = 220 \text{ K}$
$V = 772.0 (3) \text{ \AA}^3$	Plate, colourless
$Z = 2$	$0.12 \times 0.06 \times 0.03 \text{ mm}$
Bruker APEX-II CCD diffractometer	857 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{\text{int}} = 0.083$

Absorption correction: multi-scan <i>SADABS2014/5</i> (Bruker,2014/5) was used for absorption correction. <i>wR2(int)</i> was 0.0746 before and 0.0561 after correction. The Ratio of minimum to maximum transmission is 0.9221. The $\lambda/2$ correction factor is 0.00150.	$\theta_{\max} = 27.2^\circ$, $\theta_{\min} = 2.4^\circ$
$T_{\min} = 0.687$, $T_{\max} = 0.746$	$h = -11 \rightarrow 11$
6195 measured reflections	$k = -11 \rightarrow 11$
1710 independent reflections	$l = -12 \rightarrow 12$
Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.084$	$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{\max} < 0.001$
1710 reflections	$\Delta)_{\max} = 0.95 \text{ e } \text{\AA}^{-3}$
122 parameters	$\Delta)_{\min} = -0.86 \text{ e } \text{\AA}^{-3}$
0 restraints	

Table S8. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for $[\text{Ag}_3(\text{N}_5)_4]_n \cdot n[\text{Ag}(\text{NH}_3)_2]$

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	1.000000	0.500000	0.500000	0.0287 (3)
Ag3	0.500000	1.000000	0.500000	0.0322 (3)
Ag2	0.25565 (9)	0.66969 (6)	0.25037 (11)	0.0317 (2)
N1	0.4871 (8)	0.5383 (7)	0.3416 (8)	0.0231 (17)
N2	0.6261 (8)	0.5879 (7)	0.4086 (8)	0.0239 (18)
N3	0.7248 (8)	0.4807 (7)	0.4176 (8)	0.0246 (17)
N4	0.6469 (7)	0.3632 (7)	0.3540 (8)	0.0244 (18)
N5	0.4956 (9)	0.3979 (8)	0.3050 (9)	0.029 (2)
N6	0.0747 (8)	0.8011 (7)	0.3250 (8)	0.0247 (18)
N7	0.0017 (9)	0.7595 (7)	0.4154 (8)	0.0270 (18)
N8	-0.1077 (8)	0.8574 (7)	0.4089 (9)	0.0291 (19)
N9	-0.1007 (8)	0.9592 (8)	0.3170 (8)	0.0245 (17)
N10	0.0139 (8)	0.9259 (7)	0.2678 (9)	0.0234 (19)
N11	0.6862 (8)	0.8595 (7)	0.6031 (8)	0.0284 (18)
H11A	0.716977	0.811875	0.536911	0.034*
H11B	0.655417	0.793812	0.656721	0.034*
H11C	0.765825	0.912661	0.659913	0.034*

Table S9. Atomic displacement parameters (\AA^2) for $[\text{Ag}_3(\text{N}_5)_4]_n \cdot n[\text{Ag}(\text{NH}_3)_2]$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0183 (6)	0.0268 (6)	0.0396 (8)	-0.0020 (5)	0.0073 (5)	0.0046 (6)
Ag3	0.0352 (7)	0.0327 (7)	0.0315 (7)	0.0006 (5)	0.0148 (6)	-0.0015 (6)
Ag2	0.0205 (3)	0.0171 (3)	0.0618 (5)	0.0020 (4)	0.0195 (3)	0.0049 (5)
N1	0.020 (4)	0.021 (4)	0.033 (5)	0.003 (3)	0.014 (4)	0.002 (3)
N2	0.017 (4)	0.018 (4)	0.038 (5)	0.003 (3)	0.012 (4)	0.001 (4)
N3	0.022 (4)	0.021 (4)	0.032 (5)	0.003 (3)	0.011 (4)	-0.005 (4)
N4	0.009 (4)	0.023 (4)	0.042 (5)	0.003 (3)	0.011 (4)	0.002 (4)
N5	0.023 (4)	0.020 (4)	0.043 (6)	-0.005 (3)	0.011 (4)	0.006 (4)
N6	0.015 (4)	0.020 (4)	0.040 (5)	0.002 (3)	0.010 (4)	0.006 (4)
N7	0.035 (5)	0.017 (4)	0.033 (5)	0.008 (3)	0.017 (4)	0.011 (4)
N8	0.028 (4)	0.018 (4)	0.046 (5)	0.000 (3)	0.019 (4)	0.008 (4)
N9	0.013 (4)	0.027 (4)	0.037 (5)	0.004 (3)	0.012 (4)	-0.005 (4)
N10	0.020 (4)	0.017 (4)	0.037 (5)	-0.001 (3)	0.015 (4)	0.003 (4)
N11	0.031 (4)	0.021 (4)	0.038 (5)	-0.011 (3)	0.019 (4)	-0.004 (4)

Table S10. Geometric parameters (\AA , $^\circ$) for $[\text{Ag}_3(\text{N}_5)_4]_n \cdot n[\text{Ag}(\text{NH}_3)_2]$

Ag1—N3	2.375 (7)	N1—N5	1.338 (9)
Ag1—N3 ⁱ	2.375 (7)	N2—N3	1.310 (8)
Ag1—N7 ⁱⁱ	2.507 (6)	N3—N4	1.324 (9)
Ag1—N7 ⁱⁱⁱ	2.507 (6)	N4—N5	1.340 (9)
Ag1—N10 ^{iv}	2.686 (8)	N6—N7	1.327 (9)
Ag1—N10 ^v	2.686 (8)	N6—N10	1.309 (9)
Ag3—N11 ^{vi}	2.103 (7)	N7—N8	1.322 (9)
Ag3—N11	2.103 (7)	N8—N9	1.311 (9)
Ag2—N1	2.334 (7)	N9—N10	1.318 (9)
Ag2—N4 ^{vii}	2.353 (7)	N11—H11A	0.9000
Ag2—N6	2.337 (7)	N11—H11B	0.9000
Ag2—N9 ^{viii}	2.345 (7)	N11—H11C	0.9000
N1—N2	1.303 (9)		
N3—Ag1—N3 ⁱ	180.0	N1—N2—N3	107.9 (6)
N3 ⁱ —Ag1—N7 ⁱⁱⁱ	85.7 (2)	N2—N3—Ag1	126.3 (5)
N3—Ag1—N7 ⁱⁱⁱ	94.3 (2)	N2—N3—N4	108.7 (7)
N3 ⁱ —Ag1—N7 ⁱⁱ	94.3 (2)	N4—N3—Ag1	124.4 (5)
N3—Ag1—N7 ⁱⁱ	85.7 (2)	N3—N4—Ag2 ^{iv}	126.4 (5)
N3—Ag1—N10 ^{iv}	86.3 (2)	N3—N4—N5	108.1 (6)

N3 ⁱ —Ag1—N10 ^v	86.3 (2)	N5—N4—Ag2 ^{iv}	120.4 (6)
N3 ⁱ —Ag1—N10 ^{iv}	93.7 (2)	N1—N5—N4	105.7 (7)
N3—Ag1—N10 ^v	93.7 (2)	N7—N6—Ag2	128.4 (5)
N7 ⁱⁱ —Ag1—N7 ⁱⁱⁱ	180.0	N10—N6—Ag2	123.5 (6)
N7 ⁱⁱ —Ag1—N10 ^v	85.1 (2)	N10—N6—N7	107.6 (7)
N7 ⁱⁱⁱ —Ag1—N10 ^v	94.9 (2)	N6—N7—Ag1 ^{ix}	123.4 (5)
N7 ⁱⁱ —Ag1—N10 ^{iv}	94.9 (2)	N8—N7—Ag1 ^{ix}	124.5 (5)
N7 ⁱⁱⁱ —Ag1—N10 ^{iv}	85.1 (2)	N8—N7—N6	107.8 (6)
N10 ^{iv} —Ag1—N10 ^v	180.0	N9—N8—N7	107.9 (7)
N11 ^{vi} —Ag3—N11	180.0	N8—N9—Ag2 ^x	127.9 (5)
N1—Ag2—N4 ^{vii}	97.6 (2)	N8—N9—N10	108.2 (7)
N1—Ag2—N6	141.3 (3)	N10—N9—Ag2 ^x	123.9 (6)
N1—Ag2—N9 ^{viii}	94.3 (3)	N6—N10—N9	108.4 (7)
N6—Ag2—N4 ^{vii}	99.0 (2)	Ag3—N11—H11A	109.5
N6—Ag2—N9 ^{viii}	95.1 (2)	Ag3—N11—H11B	109.5
N9 ^{viii} —Ag2—N4 ^{vii}	139.9 (3)	Ag3—N11—H11C	109.5
N2—N1—Ag2	128.6 (5)	H11A—N11—H11B	109.5
N2—N1—N5	109.7 (6)	H11A—N11—H11C	109.5
N5—N1—Ag2	120.6 (6)	H11B—N11—H11C	109.5
Ag1—N3—N4—Ag2 ^{iv}	-17.3 (10)	N2—N1—N5—N4	0.5 (10)
Ag1—N3—N4—N5	-171.7 (5)	N2—N3—N4—Ag2 ^{iv}	154.0 (6)
Ag1 ^{ix} —N7—N8—N9	-158.3 (5)	N2—N3—N4—N5	-0.4 (10)
Ag2—N1—N2—N3	-168.9 (5)	N3—N4—N5—N1	0.0 (9)
Ag2—N1—N5—N4	169.7 (5)	N5—N1—N2—N3	-0.7 (10)
Ag2 ^{iv} —N4—N5—N1	-156.2 (5)	N6—N7—N8—N9	-0.9 (9)
Ag2—N6—N7—Ag1 ^{ix}	-12.3 (10)	N7—N6—N10—N9	-2.7 (9)
Ag2—N6—N7—N8	-170.1 (6)	N7—N8—N9—Ag2 ^x	-179.5 (6)
Ag2—N6—N10—N9	170.0 (5)	N7—N8—N9—N10	-0.8 (9)
Ag2 ^x —N9—N10—N6	-179.1 (5)	N8—N9—N10—N6	2.2 (9)
N1—N2—N3—Ag1	171.8 (5)	N10—N6—N7—Ag1 ^{ix}	159.9 (5)
N1—N2—N3—N4	0.7 (10)	N10—N6—N7—N8	2.2 (9)

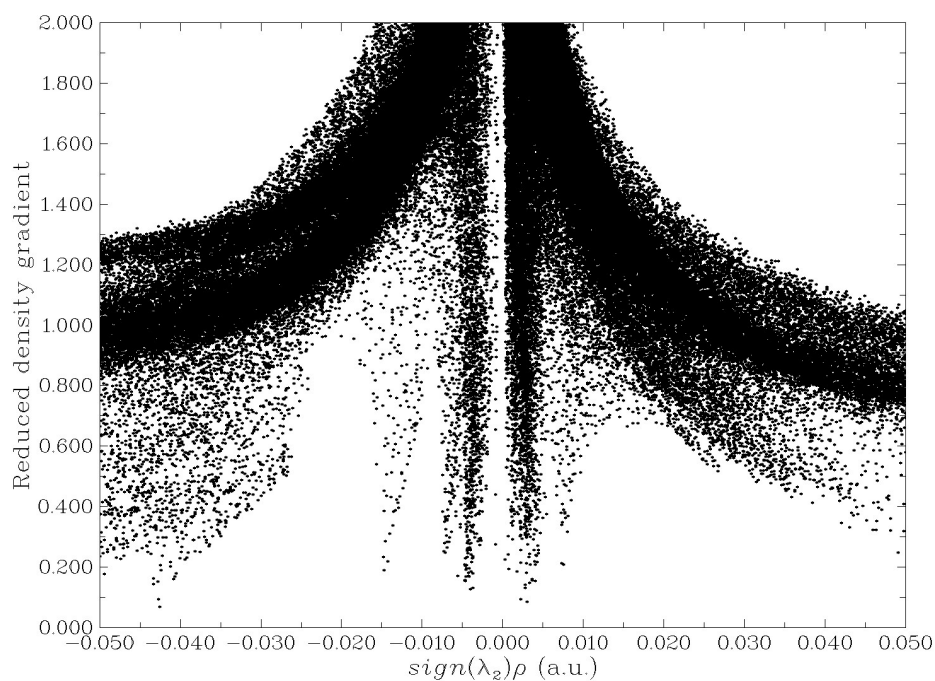
Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x+1, y, z$; (iv) $-x+1, y-1/2, -z+1/2$; (v) $x+1, -y+3/2, z+1/2$; (vi) $-x+1, -y+2, -z+1$; (vii) $-x+1, y+1/2, -z+1/2$; (viii) $-x, y-1/2, -z+1/2$; (ix) $x-1, y, z$; (x) $-x, y+1/2, -z+1/2$.

Table S11. Hydrogen bonds (Å, °) for $[\text{Ag}_3(\text{N}_5)_4]_n \cdot n[\text{Ag}(\text{NH}_3)_2]$

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N11—H11A \cdots N2	0.90	2.40	3.068 (10)	131
N11—H11A \cdots N8 ⁱⁱⁱ	0.90	2.37	3.081 (10)	136
N11—H11B \cdots N5 ⁱⁱ	0.90	2.33	3.164 (9)	155
N11—H11C \cdots N3 ^{xi}	0.90	2.85	3.337 (10)	115
N11—H11C \cdots N10 ^{vi}	0.90	2.40	3.261 (10)	160

Symmetry codes: (ii) $-x+1, -y+1, -z+1$; (iii) $x+1, y, z$; (vi) $-x+1, -y+2, -z+1$; (xi) $x, -y+3/2, z+1/2$.

4. The noncovalent interactions study

**Fig. S1** Plots of the reduced density gradient versus the electron density multiplied by the sign of the second Hessian eigenvalue for $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$.

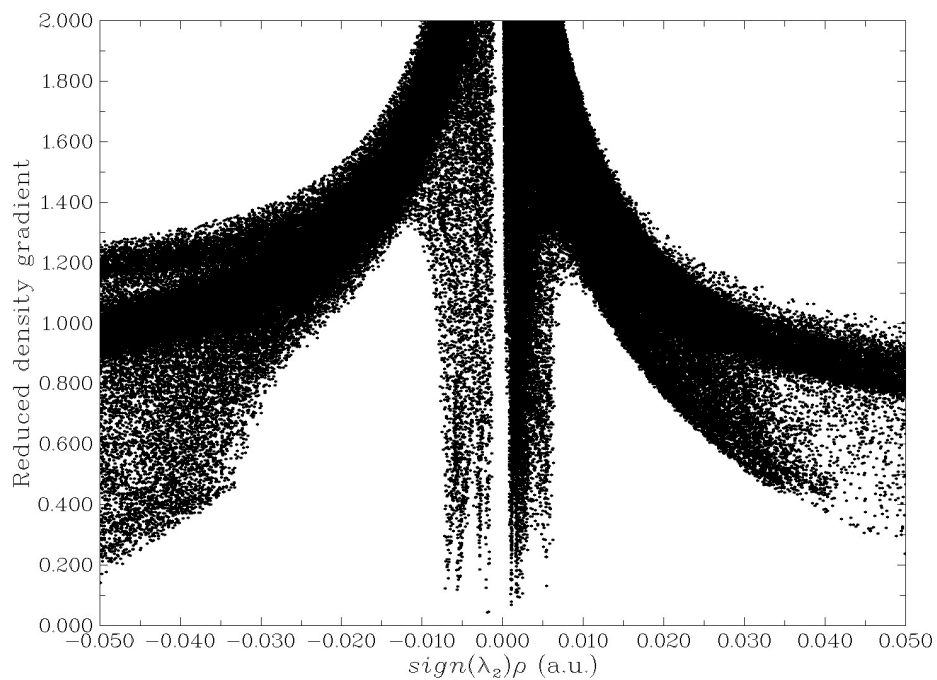


Fig. S2 Plots of the reduced density gradient versus the electron density multiplied by the sign of the second Hessian eigenvalue for $[Ag(N_5)]_n$.

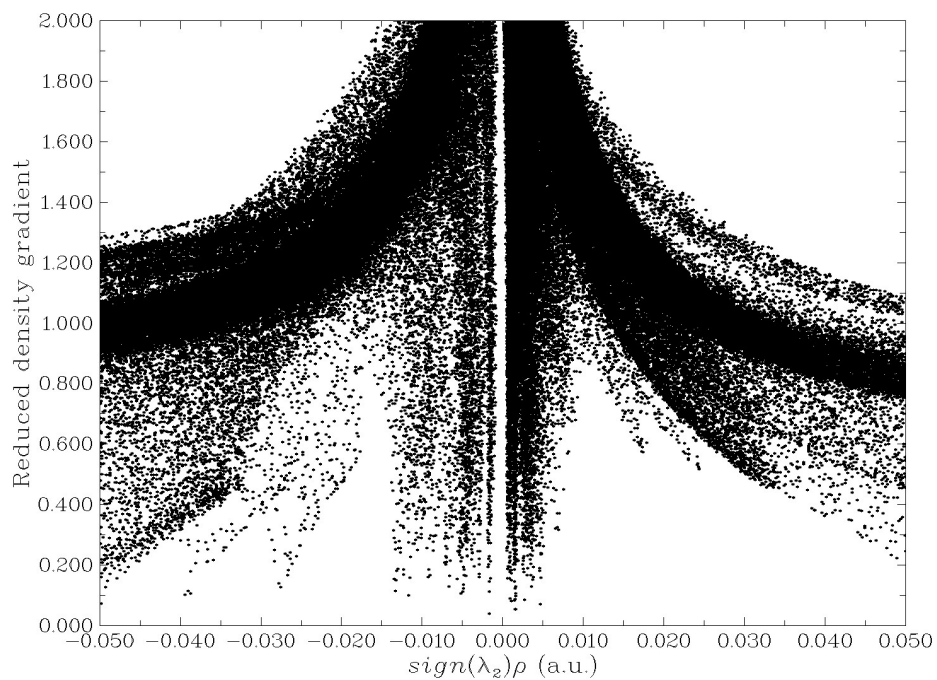


Fig. S3 Plots of the reduced density gradient versus the electron density multiplied by the sign of the second Hessian eigenvalue for $[Ag_3(N_5)_4]_n \cdot n[Ag(NH_3)_2]$.

5. IR spectrum

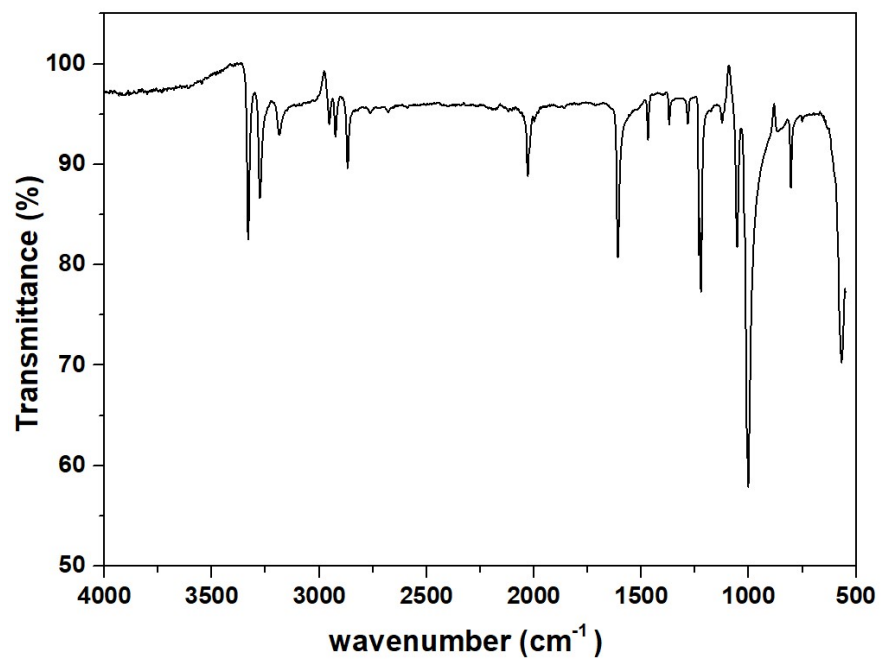


Fig. S4 The IR spectrum of $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$.

6. TG curve

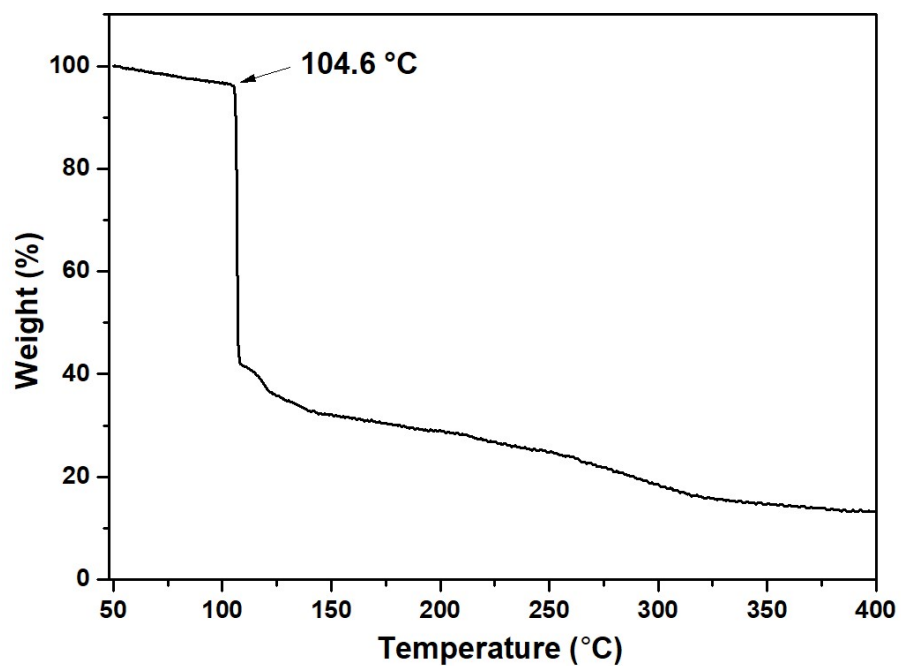


Fig. S5 The TG curve of $[\text{Ag}_2(\text{N}_5)_2(\text{EDA})]_n$.

Reference

- 1 Y. Xu, Q. Lin, P. Wang and M. Lu, *Chem. -Asian J.*, 2018, **13**, 1669-1673.