Electronic supplementary information (ESI)

Guest-containing supramolecular isomers of silver(I) 3,5-dialkyl-1,2,4-triazolates: syntheses, structures, and transformation behaviours †

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Table S1. Selected bond lengths (Å) and angles (°), as well as short contacts (Å).

2b[a]		**2b'**[b]		**4c**[c]	
Ag1-N3A	2.161(3)	Ag1-N15A	2.194(2)	Ag1-N2A	2.238(6)
Ag1-N3	2.161(3)	Ag1-N4B	2.194(2)	Ag1-N1B	2.251(4)
Ag1-N1	2.309(4)	Ag1-N1	2.376(2)	Ag1-N1	2.251(4)
Ag2-N6	2.195(3)	Ag2-N2	2.163(2)	N1-C1	1.333(7)
Ag2-N5	2.214(3)	Ag2-N10	2.169(2)	N1-N1C	1.396(9)
Ag2-N7B	2.273(3)	Ag2-N6	2.315(2)	N2-C1C	1.353(6)
Ag3-N8C	2.170(3)	Ag3-N9	2.162(2)	N2-C1	1.353(6)
Ag3-N2D	2.187(3)	Ag3-N5B	2.177(2)	N2-Ag1D	2.238(6)
Ag3-N4	2.356(3)	Ag3-N11	2.380(2)		
N2-Ag3E	2.187(3)	Ag4-N8C	2.216(2)	Ag1···H4E	2.75(1)
N7-Ag2B	2.273(3)	Ag4-N12	2.222(2)	C7···H6	2.82(1)
N8-Ag3F	2.170(3)	Ag4-N13	2.242(2)	H7···H7F	2.34(2)
		Ag5-N14	2.195(2)		
		Ag5-N3D	2.214(2)		
		Ag5-N7C	2.282(2)		
		N3-Ag5E	2.214(2)		
		N4-Ag1F	2.194(2)		
		N5-Ag3F	2.177(2)		
		N7-Ag5G	2.282(2)		
		N8-Ag4G	2.216(2)		
		N15-Ag1H	2.194(2)		
N3A-Ag1-N3	138.64(16)	N15A-Ag1-N4B	140.90(8)	N2A-Ag1-N1B	122.96(11)
N3A-Ag1-N1	110.68(8)	N15A-Ag1-N1	111.19(8)	N2A-Ag1-N1	122.96(11)
N3-Ag1-N1	110.68(8)	N4B-Ag1-N1	106.61(8)	N1B-Ag1-N1	114.1(2)
N6-Ag2-N5	130.08(12)	N2-Ag2-N10	139.80(9)		
N6-Ag2-N7B	115.76(10)	N2-Ag2-N6	111.32(8)		
N5-Ag2-N7B	114.14(12)	N10-Ag2-N6	108.81(9)		
N8C-Ag3-N2D	141.57(12)	N9-Ag3-N5B	144.50(8)		
N8C-Ag3-N4	114.51(12)	N9-Ag3-N11	117.31(9)		
N2D-Ag3-N4	102.07(12)	N5B-Ag3-N11	95.78(9)		
		N8C-Ag4-N12	124.29(9)		
		N8C-Ag4-N13	116.77(9)		
		N12-Ag4-N13	118.64(9)		
		N14-Ag5-N3D	131.22(8)		
		N14-Ag5-N7C	115.55(9)		
		N3D-Ag5-N7C	113.16(9)		

[a, b, c] Symmetry transformations used to generate equivalent atoms:

[a]	[b]	[c]
A = -x+2,y,-z+1/2	A = x,-y+1/2,z-1/2	A = -y+1/2,-z+3/2,-x+1/2
B = -x+1,-y+1,-z+1	B = -x+1,y-1/2,-z+1/2	B = x,y,-z+1

C = x+1,y,z D = x,y+1,z E = x,y-1,z F = x-1,y,z	C = x-1,y,z D = x-1,-y+1/2,z+1/2 E = x+1,-y+1/2,z-1/2 F = -x+1,y+1/2,-z+1/2 G = x+1,y,z H = x,-y+1/2,z+1/2	C = -x,-y+1,z D = -z+1/2,-x+1/2,-y+3/2 E = 1/2+x,-1/2+y,-1/2+z F = 1+x,y,-1+z

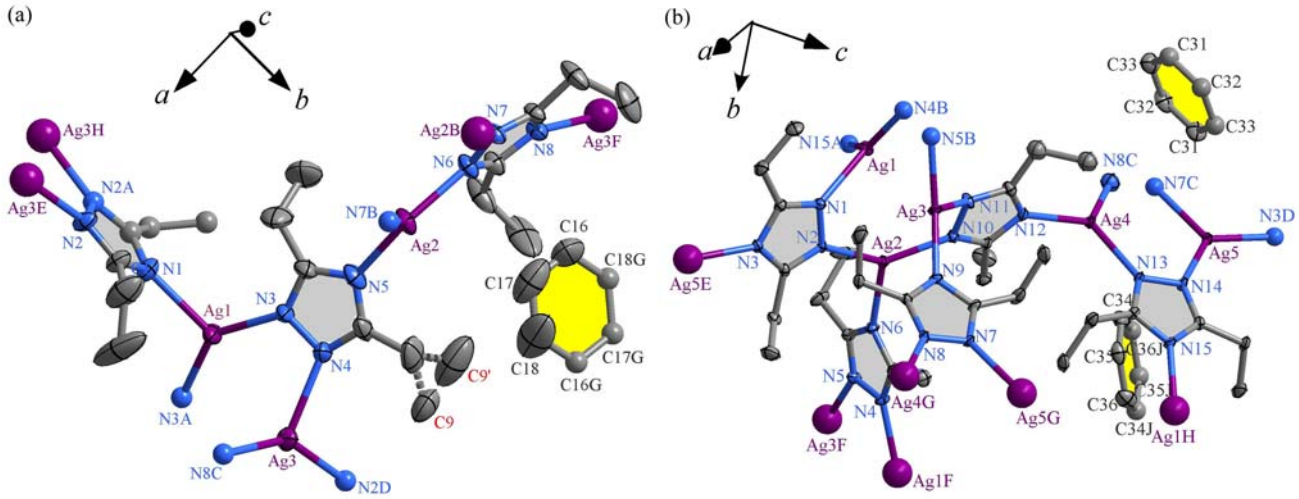

Fig. S1 Perspective view of the coordination environment of **2b** ((a), 2-fold disordered ethyl groups are shown as dashed bonds in red) and **2b'** (b) (at 50% probability; hydrogen atoms are omitted for clarity). Symmetry codes: A = 2-x, y, 0.5-z; B = -x＋1, -y＋1, 1-z; C = 1+x, y, z; D = x, 1+y, z; E = x, y-1, z; F = x-1, y, z; G = -x＋1, -y＋2, 1-z, H = 2-x, -1+y, 0.5-z for **2b**. A = x, 0.5-y, -0.5+z; B = 1-x, -0.5+y, 0.5-z; C = -1+x, y, z; D = -1+x, -y+0.5, z+0.5; E = 1+x, 0.5-y, z-0.5; F = 1-x, y+0.5, 0.5-z; G = x+1, y, z; H = x, 0.5-y, 0.5+z; I = -x, -y, 1-z; J = -x, -y+1, -z+1 for **2b'**.

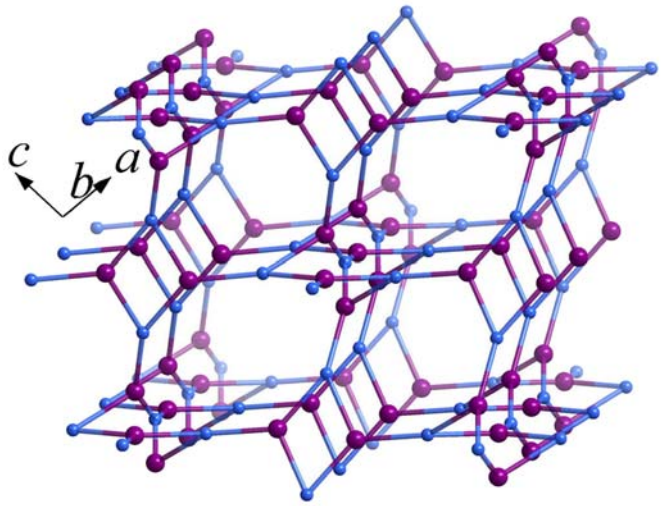

Fig. S2 The simplified topology structure of **2b/2b'** (purple and blue spheres represent the Ag ions and the triazolate ligands, two-colour sticks represent the coordination bonds.

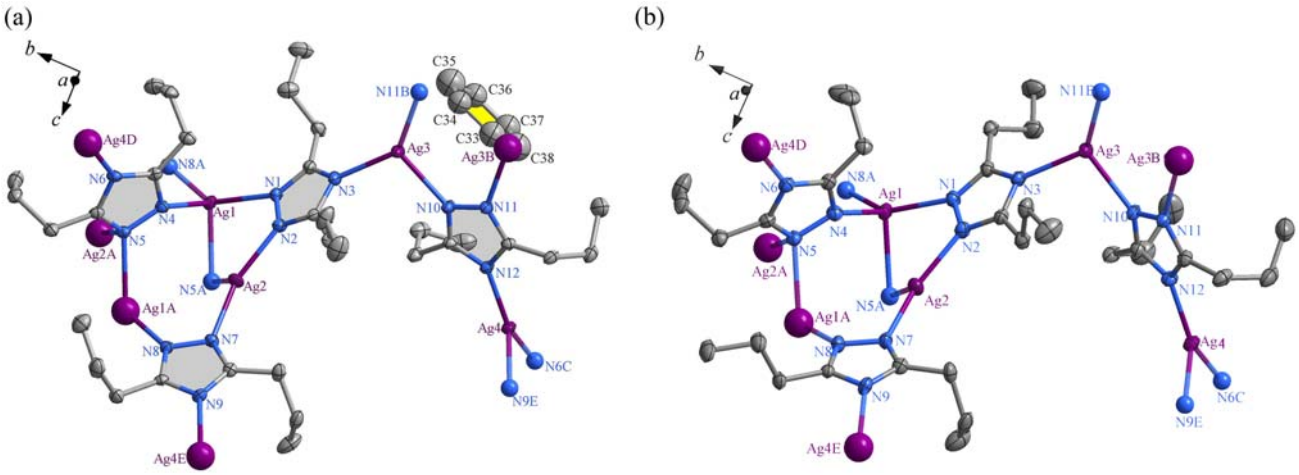

Fig. S3 Perspective view of the coordination environment of (a) **3b** and (b) **3b'** (at 50% probability; hydrogen atoms are omitted for clarity). Symmetry codes: A = 1-x, 2-y, 1-z; B = 2-x, 1-y, -z; C = x, -1+y, Z; D = x, 1+y, z; E = 2-x, 1-y, 1-z. Note that the benzene molecule in **3b** has half site occupancy.

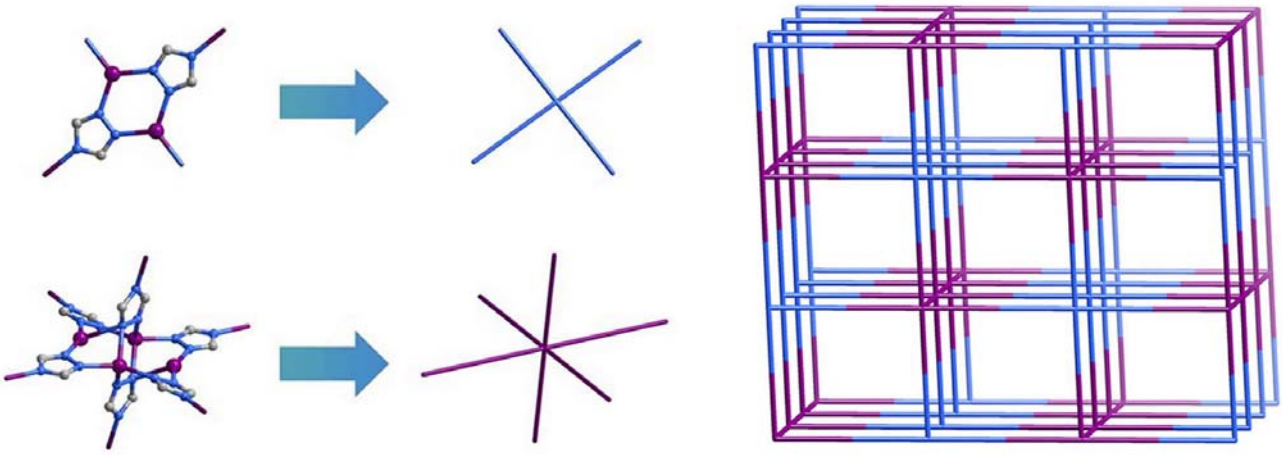

Fig. S4 The simplified topology structures of **3b/3b'**.

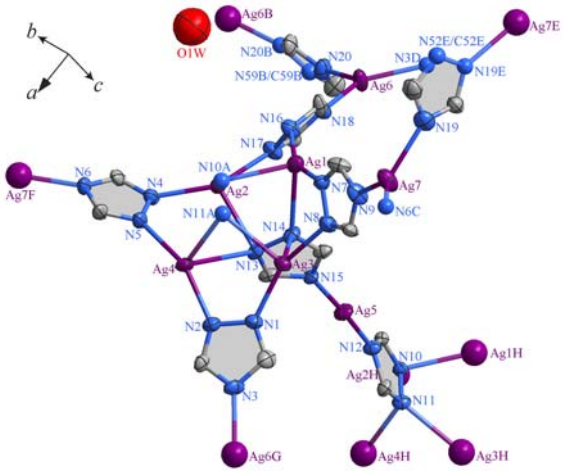

Fig. S5 Perspective view of the coordination environment of **4b** (at 50% probability; isopropyl groups are omitted for clarity). Symmetry codes: A = x, y, -1+z; B = -x, 1-y, z; C = 0.5-x, -0.5+y, -z; D = -0.5+x, 0.5-y, 1-z; E = -x, -y, z; F = 0.5-x, 0.5+y, -z; G = 0.5+x, 0.5-y, 1-z; H = x, y, 1+z.

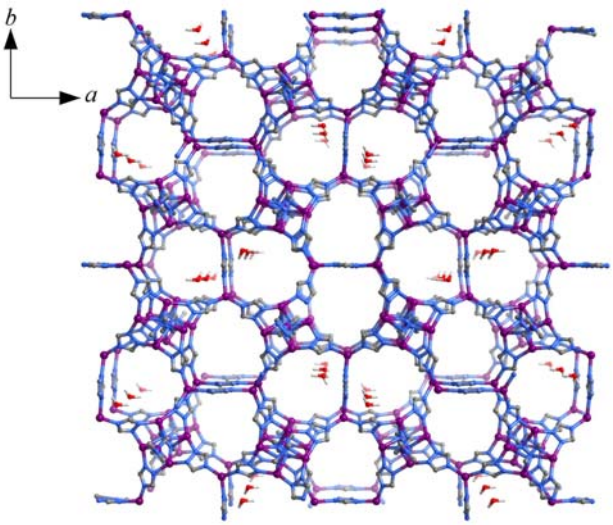

Fig. S6 Perspective view of **4b** along the *c*-axis (isopropyl groups are omitted for clarity).

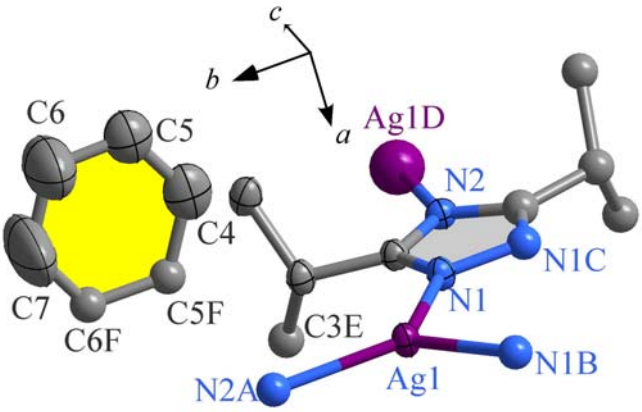

Fig. S7 Perspective view of the coordination environment of **4c** (at 50% probability; hydrogen atoms are omitted for clarity). Symmetry codes: A = x+0.5, -y+0.5, -z+1.5; B = x, y, -z+1; C = -x, 1-y, z; D = 0.5-x, 1.5-y, -0.5+z; E = -x, y, z, F = -x, y, -z+2.

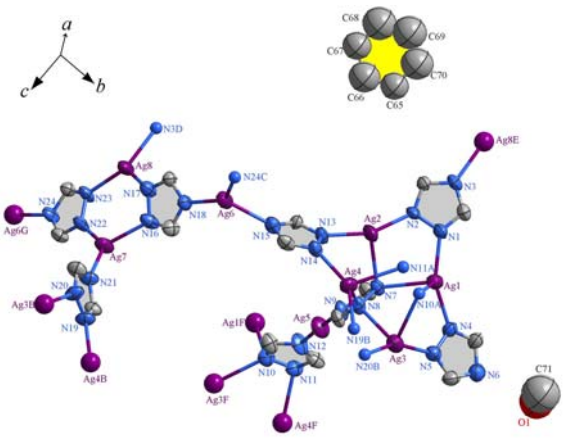

Fig. S8 Perspective view of the coordination environment of **4d** (at 50% probability; hydrogen atoms are omitted for clarity). Symmetry codes: A = -0.5+x, 1.5-y, -0.5+z; B = -x, 1-y, 1-z; C = -0.5+x, 0.5-y, -0.5+z; D = 0.5-x, -0.5+y, 0.5-z; E = 0.5-x, 0.5+y, 0.5-z; F = 0.5+x, 1.5-y, 0.5+z; G = 0.5+x, 0.5-y, 0.5+z.

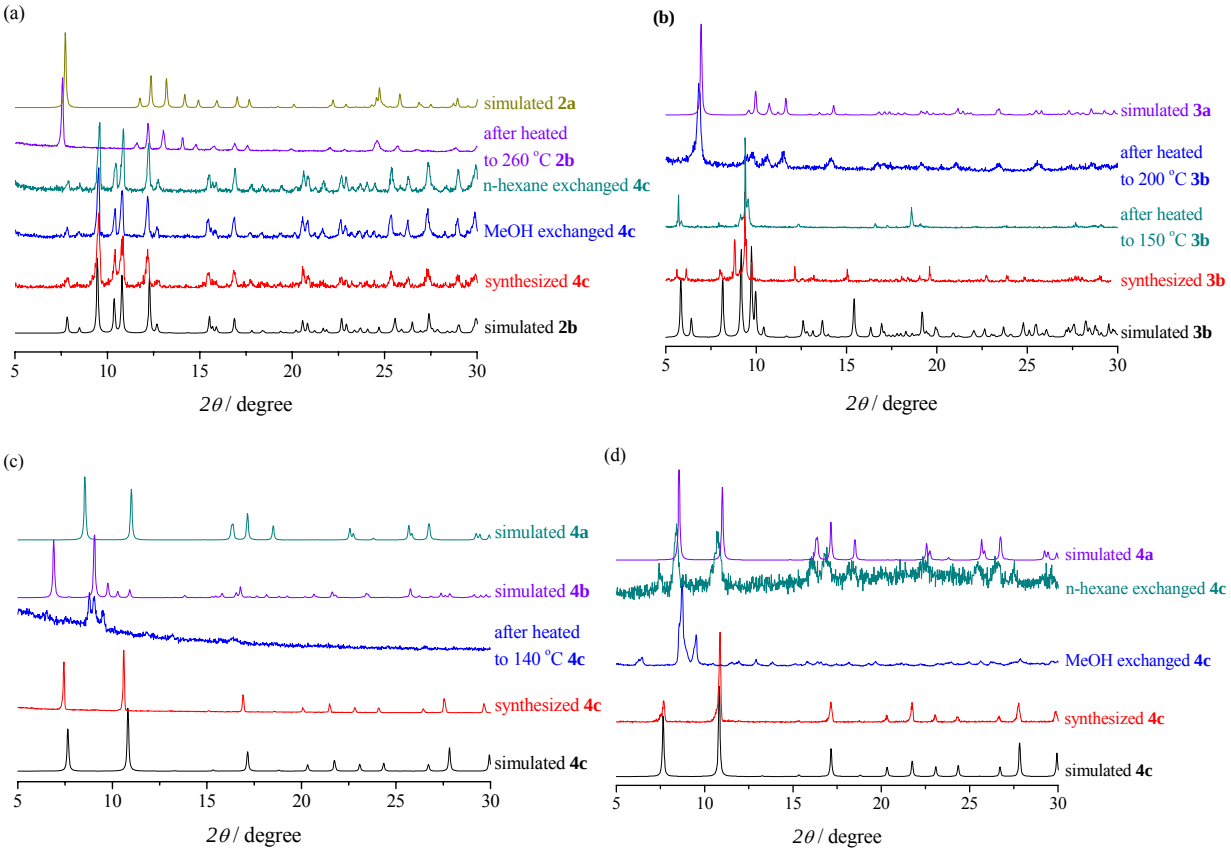

Fig. S9 PXRD patterns of the structure transformation of (a) **2b** after heated to 260 °C and immersed in methanol or n-hexane for 7 days, (b) **3b** after heated to 150 °C and 200 °C, (c) **4c** after heated to 140 °C and (d) **4c** after immersed in methanol and n-hexane for 1 day.