

Supplementary material

Single crystal to single crystal polymorphic phase tran-  
sition of a silver nitrate 24-crown-8 complex and its  
pseudo-polymorphism.

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1. Supplementary figures and tables:

Structure 1:

Atom 1	Atom 2	d 1,2 [Å]	Atom 1	Atom 2	d 1,2 [Å]
Ag1	O6	2.351(3)	Ag2	O6	2.363(4)
Ag1	O9	2.432(4)	Ag2	O4	2.395(4)
Ag1	O2	2.449(4)	Ag2	O3	2.571(4)
Ag1	O1	2.599(3)	Ag2	O13	2.58(2)
Ag1	O3	2.619(4)	Ag2	O5	2.596(3)
Ag1	O10	2.7264(5)	Ag2	O8	2.680(5)
Ag1	O7	2.751(6)	Ag2	O11	2.80(2)
Ag2	O12	2.20(3)			

Structure 1':

Atom 1	Atom 2	d 1,2 [Å]	Atom 1	Atom 2	d 1,2 [Å]
Ag1	O23	2.316(5)	Ag5	O39	2.300(5)
Ag1	O17	2.357(8)	Ag5	O29	2.366(7)

[Type text]

Ag1	O8	2.412(5)	Ag5	O10	2.404(6)
Ag1	O1	2.568(5)	Ag5	O11	2.594(5)
Ag1	O7	2.593(5)	Ag5	O9	2.643(5)
Ag1	O24	2.800(7)	Ag5	O38	2.909(7)
Ag2	O2	2.430(5)	Ag6	O35	2.342(7)
Ag2	O20	2.472(5)	Ag6	O12	2.448(7)
Ag2	O30	2.508(8)	Ag6	O33	2.517(6)
Ag2	O22	2.527(5)	Ag6	O32	2.535(5)
Ag2	O3	2.603(5)	Ag6	O13	2.629(6)
Ag2	O1	2.606(5)	Ag6	O11	2.662(5)
Ag2	O31	2.664(6)	Ag6	O37	2.862(7)
Ag3	O23	2.293(5)	Ag7	O39	2.298(5)
Ag3	O26	2.353(6)	Ag7	O36	2.402(6)
Ag3	O4	2.472(5)	Ag7	O14	2.444(5)
Ag3	O3	2.639(5)	Ag7	O13	2.584(6)
Ag3	O5	2.648(5)	Ag7	O15	2.643(5)
Ag3	O27	2.915(6)	Ag7	O37	2.847(7)
Ag3	O25	2.991(7)	Ag7	O40	2.985(8)
Ag4	O20	2.422(5)	Ag8	O16	2.396(5)
Ag4	O6	2.446(5)	Ag8	O34	2.423(5)
Ag4	O27	2.492(6)	Ag8	O18	2.481(8)
Ag4	O7	2.591(5)	Ag8	O15	2.589(5)
Ag4	O28	2.623(7)	Ag8	O9	2.634(5)
Ag4	O5	2.651(5)	Ag8	O19	2.639(7)
Ag4	O21	2.702(7)	Ag8	O32	2.641(6)

Structure 2:

Atom 1	Atom 2	d 1,2 [Å]	Atom 1	Atom 2	d 1,2 [Å]
Ag1	O6	2.453(4)	Ag2	O12	2.406(6)
Ag1	O2	2.455(3)	Ag2	O4	2.446(3)
Ag1	O9	2.485(5)	Ag2	O6	2.501(4)
Ag1	O3	2.565(3)	Ag2	O8	2.609(4)
Ag1	O1	2.617(3)	Ag2	O5	2.657(3)
Ag1	O7	2.626(5)	Ag2	O3	2.700(3)
Ag1	O10	2.699(6)	Ag2	O11	2.862(5)

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Table S1 List of all Ag-O distance until 3.05 ♦ for the three different structures.

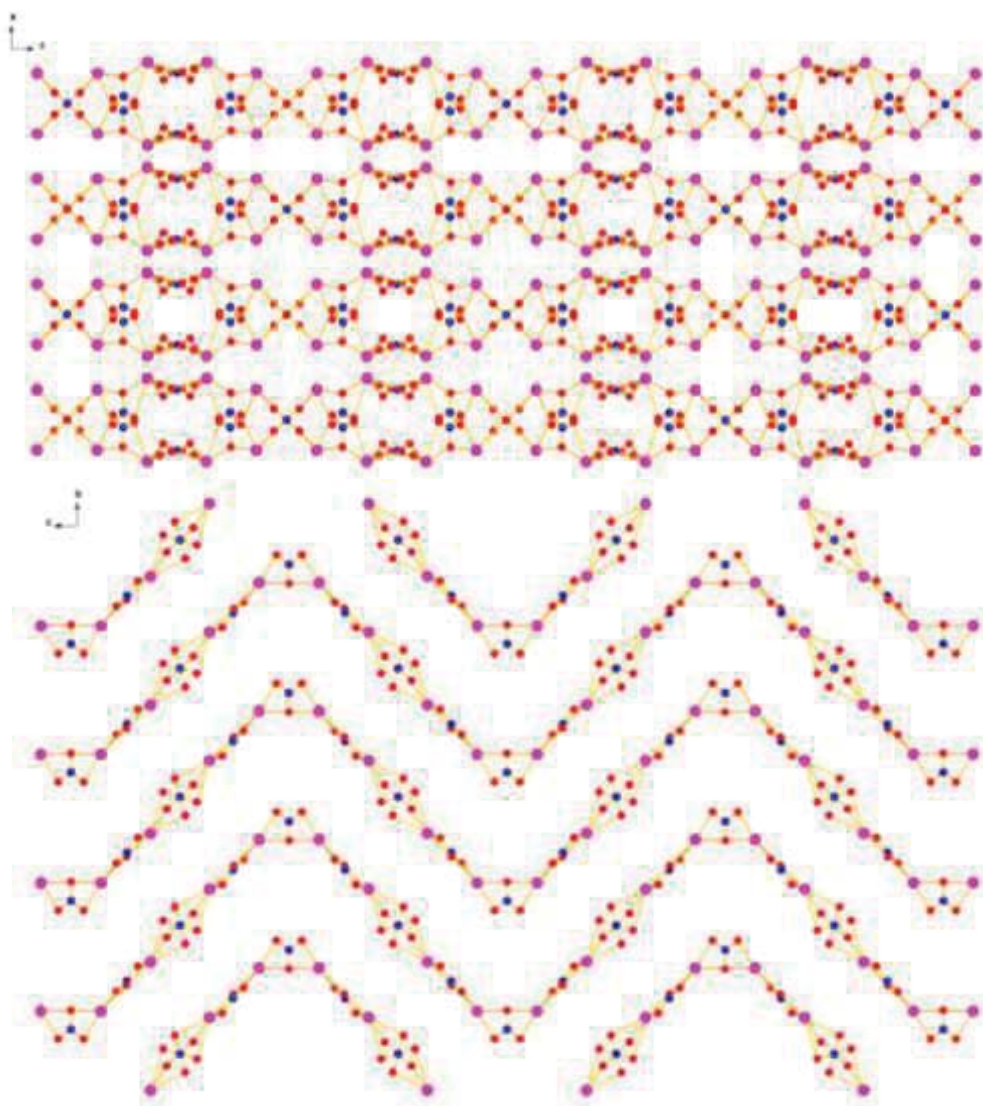


Fig. S1 Packing of the inorganic part along *b* axis (top) and view from the top of one layer (bottom) of **1**, crown ethers are omitted for clarity.

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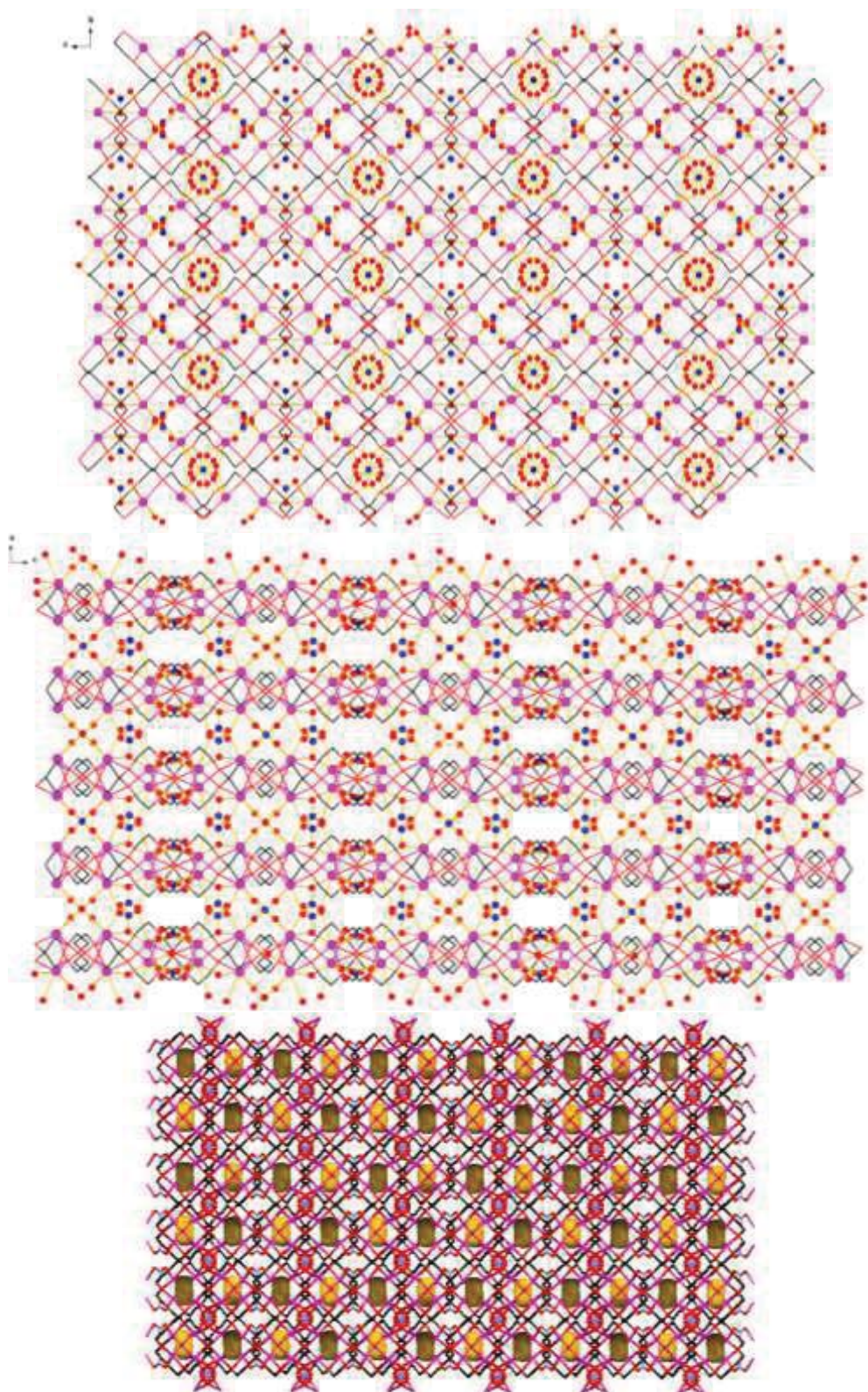


Fig. S2 Packing along *a* (top) and *b* (middle) axis of **1**, hydrogen atoms are omitted and crown ethers are shown in wire for clarity. Bottom: void calculated in the structure **1**.

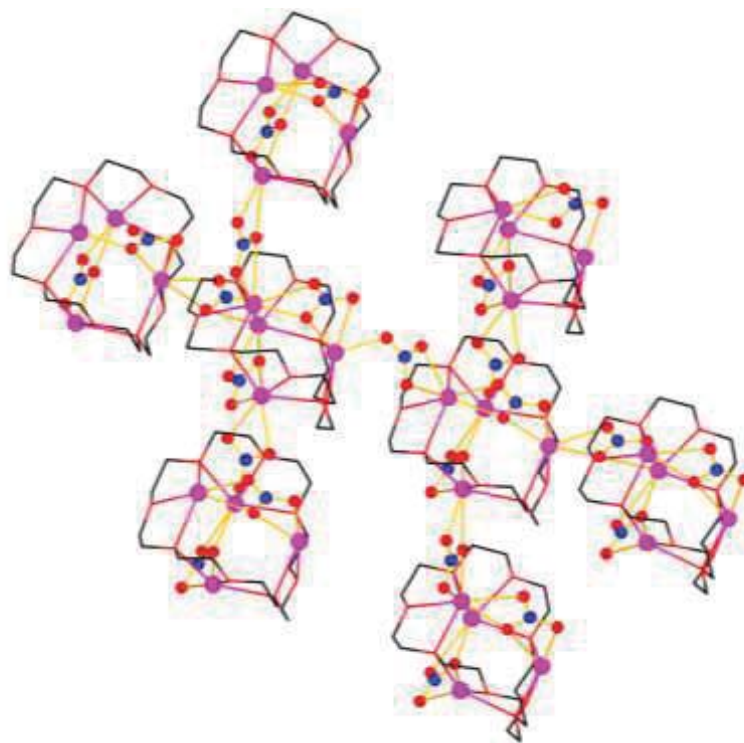


Fig. S3 View of the asymmetric unit with the neighbored crown-silver complexes. Crown ether ligands are shown in wire mode and some hydrogen atoms are omitted for clarity.



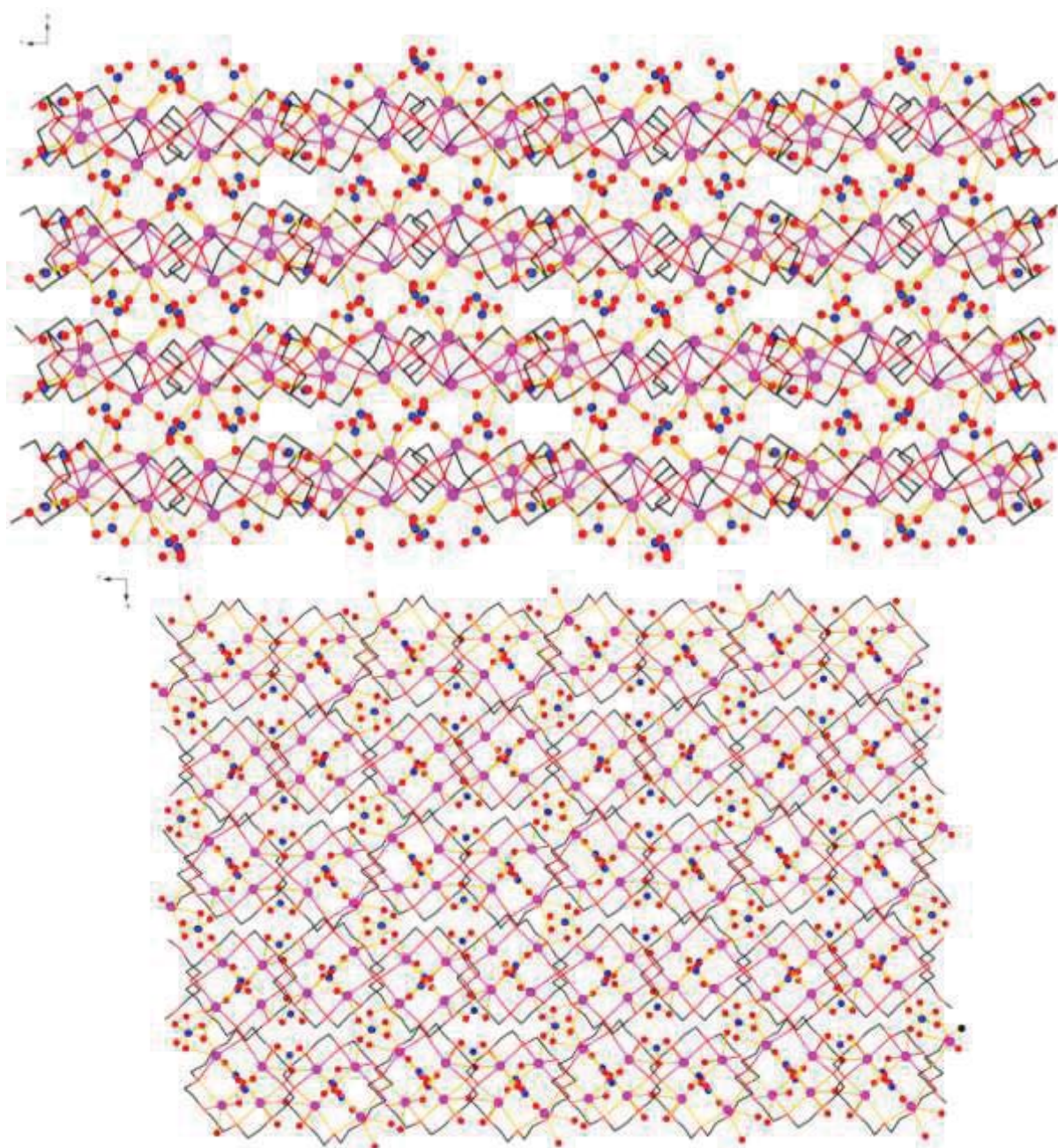


Fig. S4 Packing along *a* (top) and *b* (bottom) axis of **1'**, hydrogen atoms are omitted and crown ethers are shown in wire for clarity.

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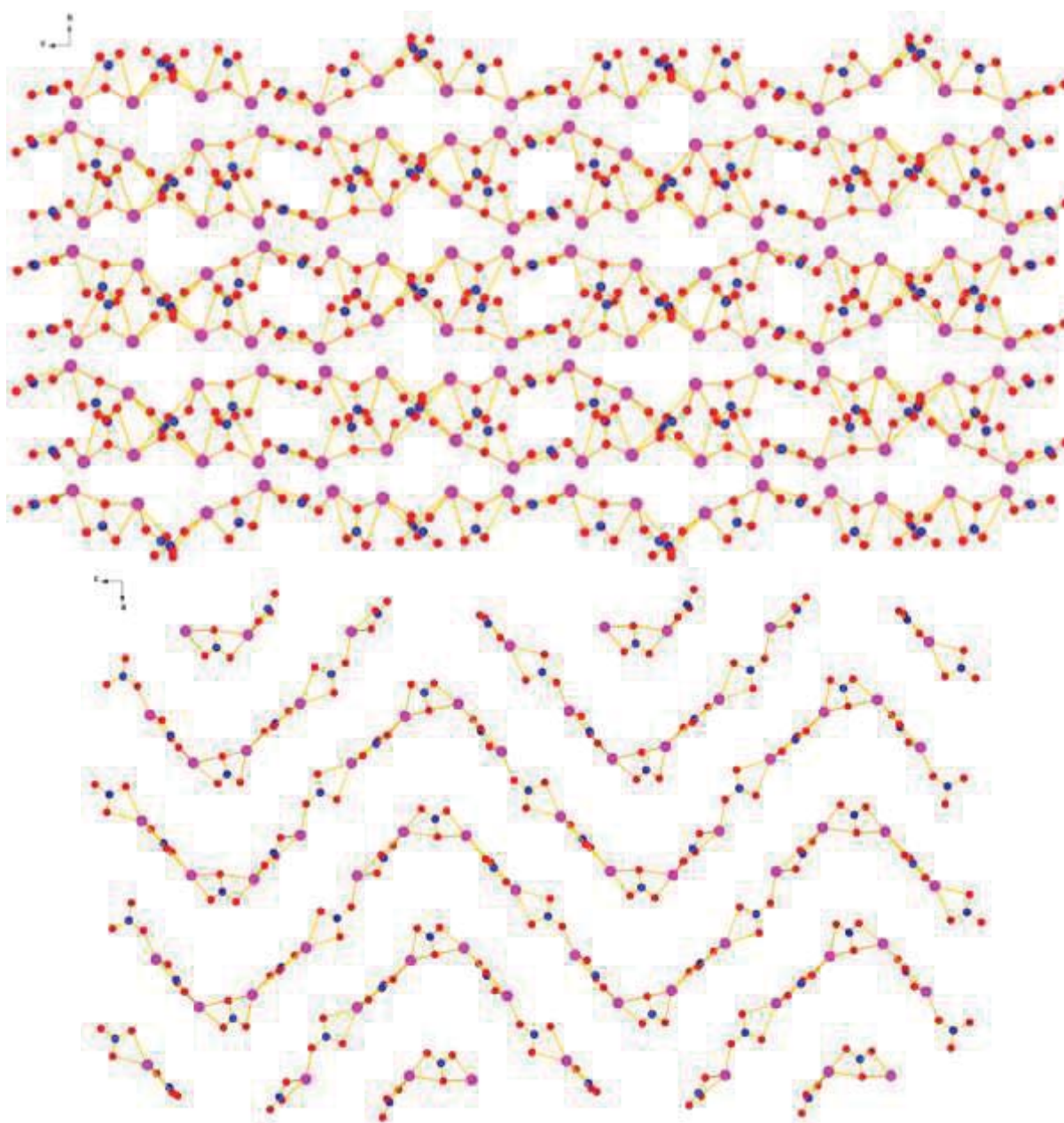


Fig. S5 Packing of the inorganic part along  $a$  axis (top) and view from the top of one layer (bottom) of **1'**, crown ethers are omitted for clarity.

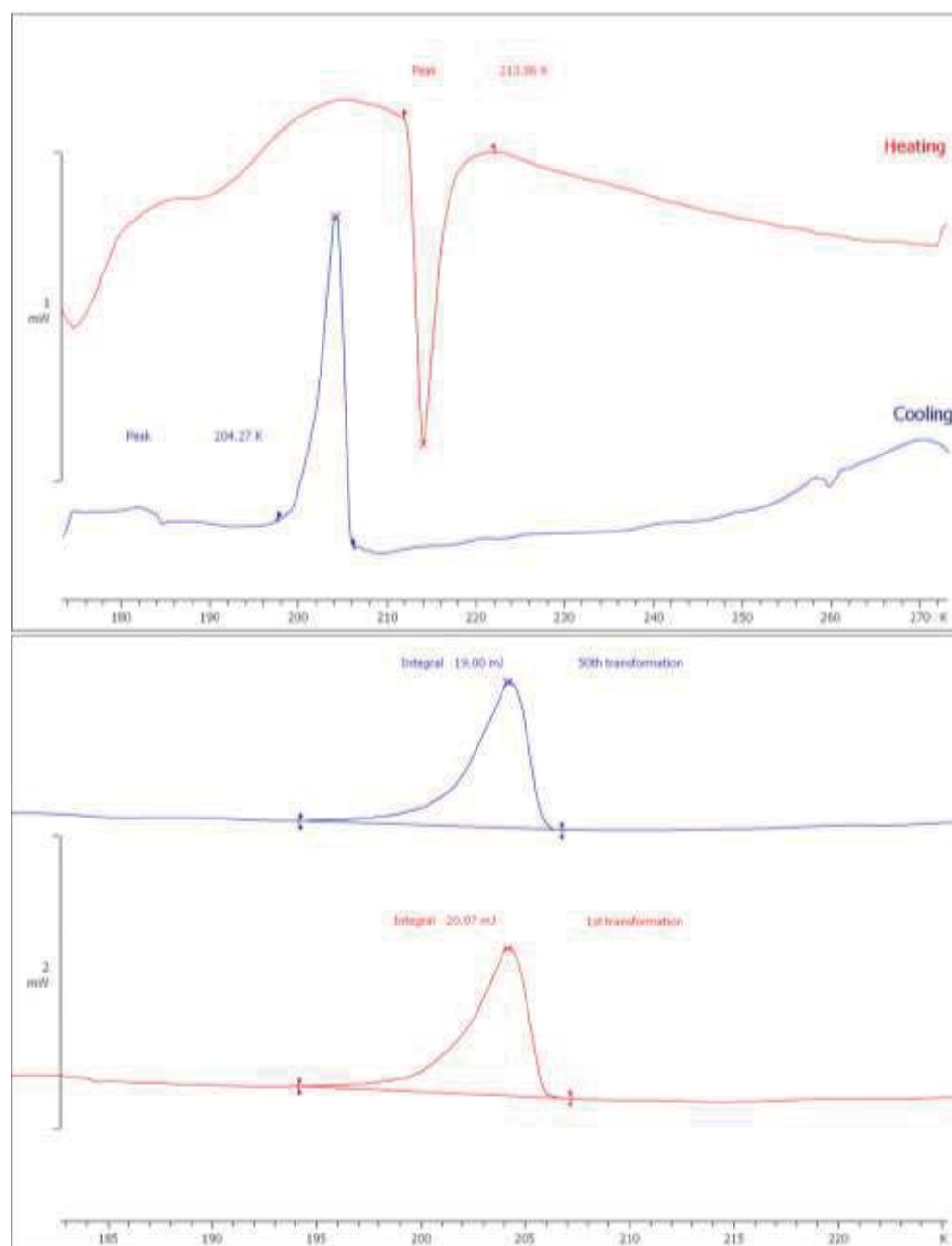


Fig. S6 DSC analysis of **1** between 170 K and 270 K (top), Comparison between the first transformation and the fiftieth one (bottom).



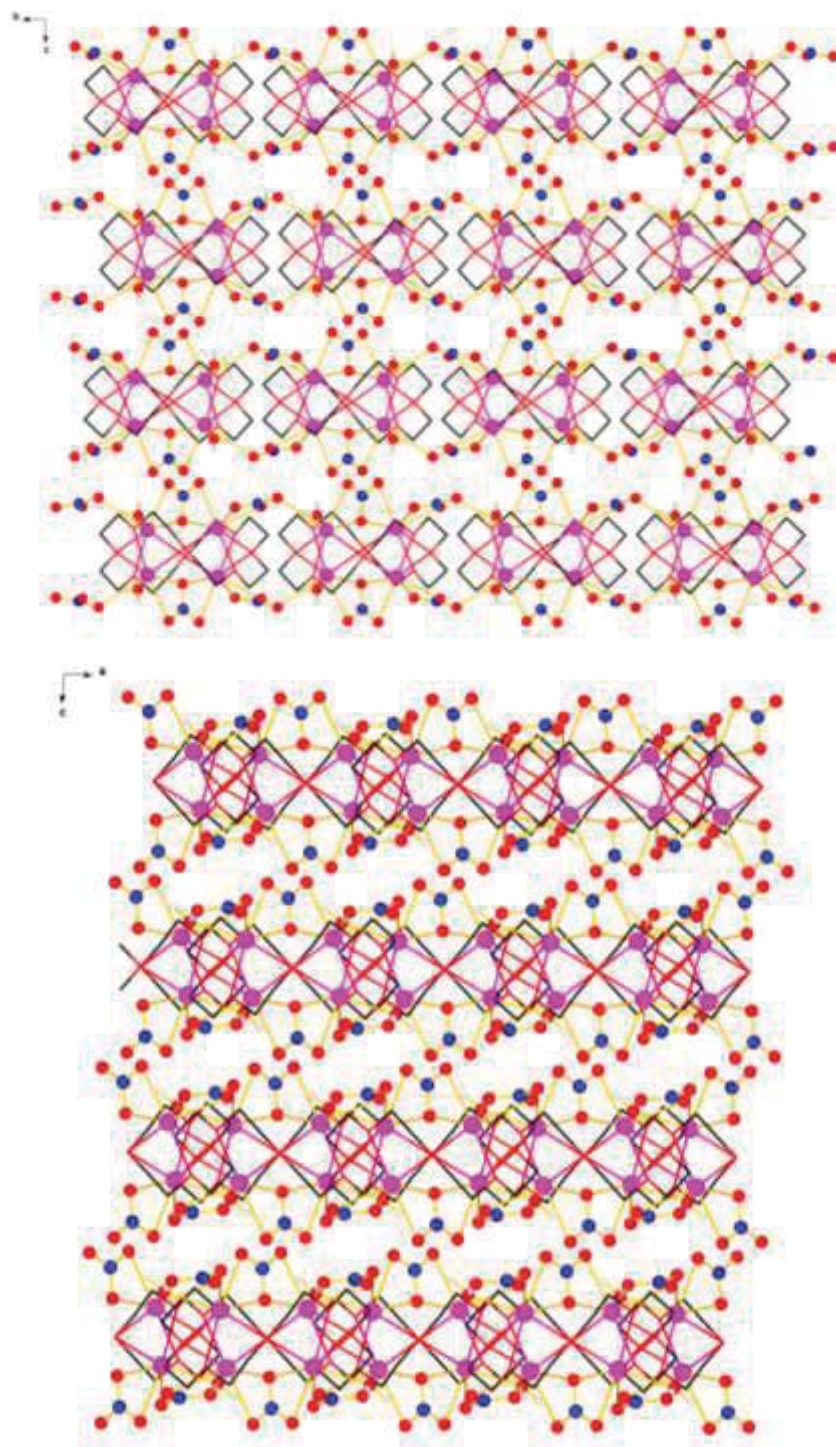


Fig. S7 Packing along *a* (top) and *b* (bottom) axis of **2**, some hydrogen atoms are omitted and crown ethers are shown in wire for clarity.

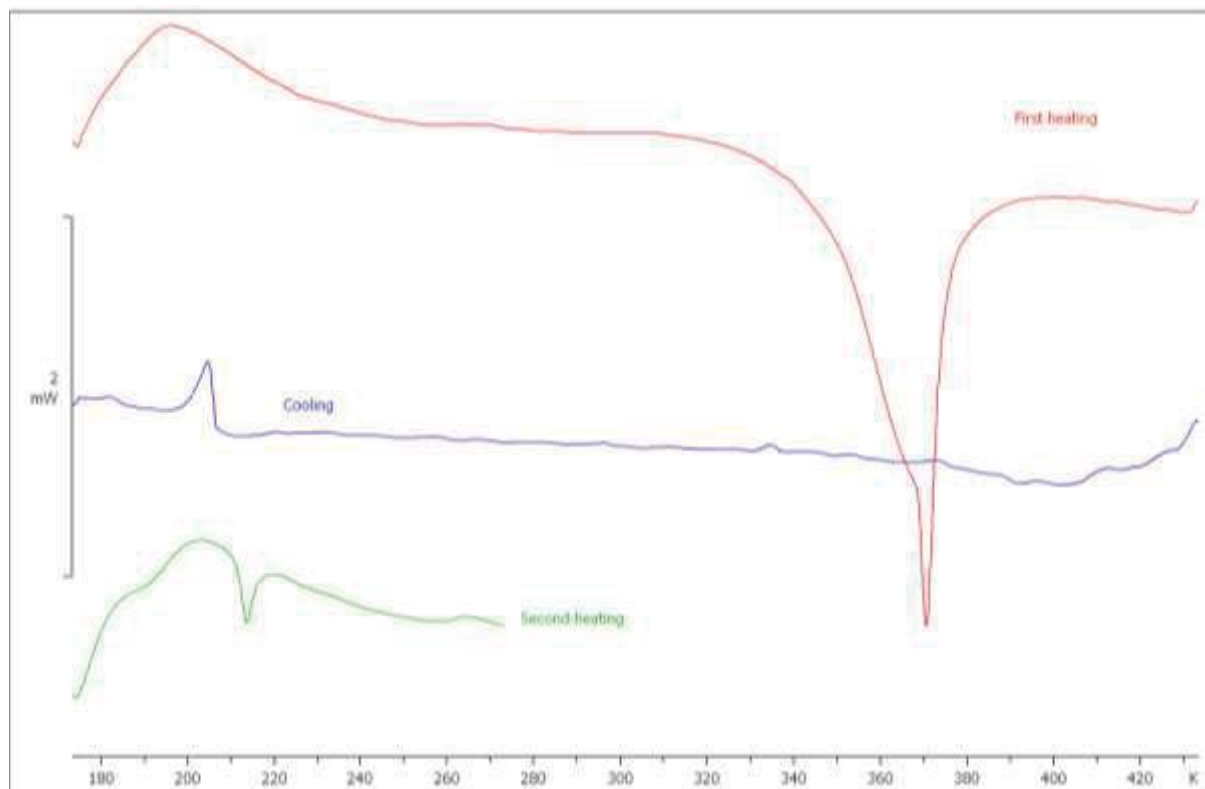


Fig. S8 DSC analysis of **2** between 170 K and 430 K.

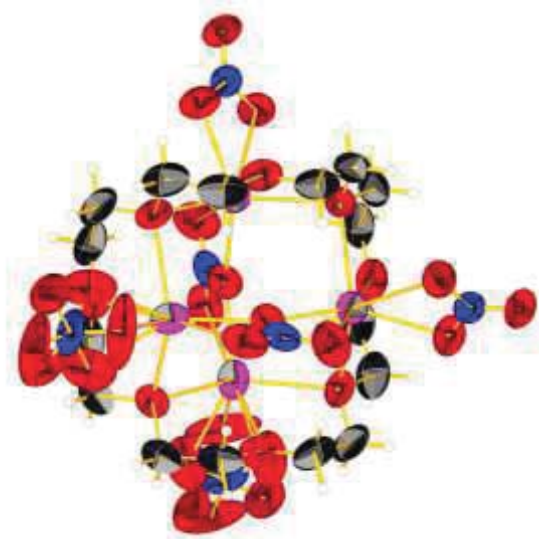


Fig. S9 Excerpt of the coordination polymer of **1** (ellipsoid probability: 50%).

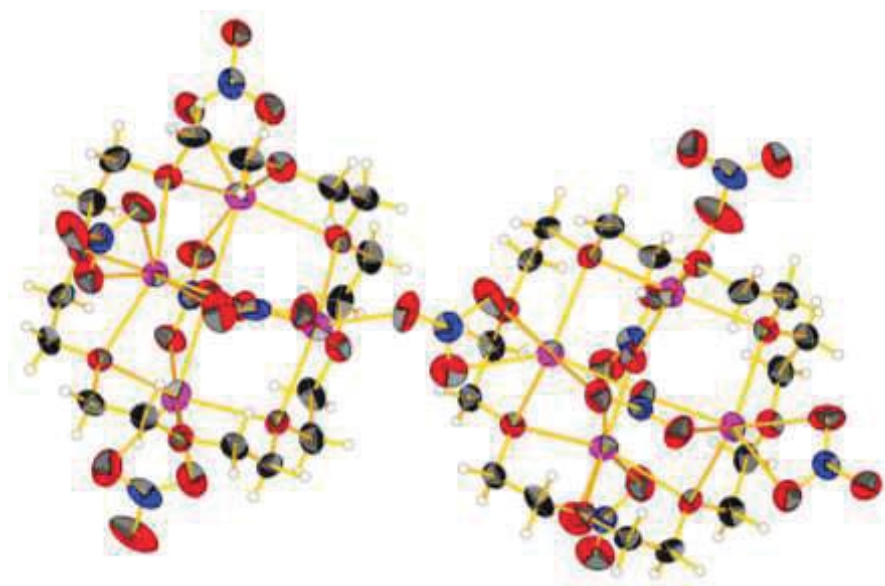


Fig. S10 Excerpt of the coordination polymer of **1'** (ellipsoid probability: 50%).

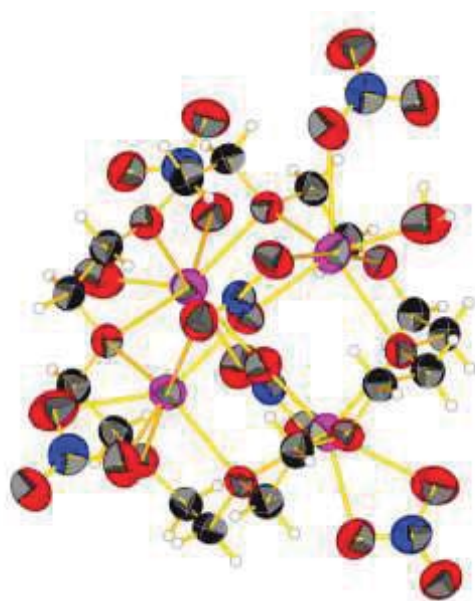


Fig. S11 Excerpt of the coordination polymer of **2** (ellipsoid probability: 50%).

## 2. Crystallographic data:

### Data for 1:



Identification code	<b>1</b>	
Empirical formula	C <sub>8</sub> H <sub>16</sub> Ag <sub>2</sub> N <sub>2</sub> O <sub>10</sub>	
Formula weight	515.97	
5 Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	<i>I</i> b c a	
Unit cell dimensions	<i>a</i> = 13.4204(6) Å	$\alpha = 90^\circ$ .
10	<i>b</i> = 16.5076(7) Å	$\beta = 90^\circ$ .
	<i>c</i> = 28.1263(13) Å	$\gamma = 90^\circ$ .
Volume	6231.1(5) Å <sup>3</sup>	
<i>Z</i>	16	
Density (calculated)	2.200 Mg/m <sup>3</sup>	
15 Absorption coefficient	2.564 mm <sup>-1</sup>	
F(000)	4032	
Crystal size	0.16 x 0.14 x 0.12 mm <sup>3</sup>	
Theta range for data collection	1.45 to 25.00°.	
Index ranges	-15 ≤ <i>h</i> ≤ 15, -19 ≤ <i>k</i> ≤ 19, -33 ≤ <i>l</i> ≤ 33	
20 Reflections collected	36758	
Independent reflections	2732 [ <i>R</i> (int) = 0.0456]	
Completeness to theta = 25.00°	99.5 %	
Absorption correction	none	
Refinement method	Full-matrix least-squares on <i>F</i> <sup>2</sup>	
25 Data / restraints / parameters	2732 / 0 / 215	
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.070	
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )]	<i>R</i> 1 = 0.0365, <i>wR</i> 2 = 0.0753	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0464, <i>wR</i> 2 = 0.0785	
Largest diff. peak and hole	1.089 and -0.601 e.Å <sup>-3</sup>	

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## Data for 1':

Identification code **1'**

Empirical formula	C32 H64 Ag8 N8 O40
Formula weight	2063.87
Temperature	200(2) K
Wavelength	0.71073 Å
5 Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	$a = 16.3286(8) \text{ Å}$ $\alpha = 90^\circ$ .
	$b = 13.4452(5) \text{ Å}$ $\beta = 90.800(4)^\circ$ .
	$c = 28.0645(14) \text{ Å}$ $\gamma = 90^\circ$ .
10 Volume	6160.7(5) Å <sup>3</sup>
Z	4
Density (calculated)	2.225 Mg/m <sup>3</sup>
Absorption coefficient	2.594 mm <sup>-1</sup>
F(000)	4032
15 Crystal size	0.19 x 0.14 x 0.13 mm <sup>3</sup>
Theta range for data collection	1.25 to 25.00°.
Index ranges	-19<= $h$ <=18, -15<= $k$ <=15, -33<= $l$ <=33
Reflections collected	40318
Independent reflections	10792 [R(int) = 0.0792]
20 Completeness to theta = 25.00°	99.5 %
Absorption correction	none
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	10792 / 0 / 793
Goodness-of-fit on F <sup>2</sup>	0.865
25 Final R indices [I>2sigma(I)]	R1 = 0.0438, wR2 = 0.0881
R indices (all data)	R1 = 0.0910, wR2 = 0.0973
Largest diff. peak and hole	0.884 and -0.739 e.Å <sup>-3</sup>

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## Data for 2:

Identification code **2**

Empirical formula	C16 H36 Ag4 N4 O22	
Formula weight	1067.97	
Temperature	273(2) K	
Wavelength	0.71073 Å	
5 Crystal system	Monoclinic	
Space group	<i>C</i> 2/c	
Unit cell dimensions	<i>a</i> = 12.1262(13) Å	$\alpha = 90^\circ$ .
	<i>b</i> = 17.6035(16) Å	$\beta = 93.461(8)^\circ$ .
	<i>c</i> = 14.7902(12) Å	$\gamma = 90^\circ$ .
10 Volume	3151.4(5) Å <sup>3</sup>	
<i>Z</i>	4	
Density (calculated)	2.251 Mg/m <sup>3</sup>	
Absorption coefficient	2.544 mm <sup>-1</sup>	
F(000)	2096	
15 Crystal size	0.27 x 0.24 x 0.23 mm <sup>3</sup>	
Theta range for data collection	2.04 to 24.99°.	
Index ranges	-14 ≤ <i>h</i> ≤ 14, -20 ≤ <i>k</i> ≤ 20, -17 ≤ <i>l</i> ≤ 17	
Reflections collected	15315	
Independent reflections	2776 [ <i>R</i> (int) = 0.0848]	
20 Completeness to theta = 24.99°	99.9 %	
Absorption correction	none	
Refinement method	Full-matrix least-squares on <i>F</i> <sup>2</sup>	
Data / restraints / parameters	2776 / 2 / 215	
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.071	
25 Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )]	<i>R</i> 1 = 0.0360, <i>wR</i> 2 = 0.0939	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0481, <i>wR</i> 2 = 0.1010	
Largest diff. peak and hole	0.752 and -1.246 e.Å <sup>-3</sup>	