Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic supplementary information

for

Influence of mole-ratio on the coordination behaviour of a ditopic $N_2O_2S_2$-macrocycle: endo/exocyclic silver(I) coordination polymer exhibiting desolvation-induced SCSC transformation

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Table S1 Crystal and experimental data

	1	**2a**	**2b**
Formula	$C_{25}H_{28}AgF_6N_2O_2PS_2$	$C_{52}H_{60}Ag_4Cl_4F_{24}N_4O_4P_4S_4$	$C_{25}H_{28}Ag_2F_{12}N_2O_2P_2S_2$
Formula weight	705.45	2086.44	958.29
Temperature	173(2)	173(2)	173(2)
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	*P*-1	*P*-1	$P2_1/c$
Z	2	2	4
a (Å)	7.9615(2)	10.6576(5)	19.6427(5)
b (Å)	11.8938(3)	17.0361(8)	10.2297(3)
c (Å)	14.6343(3)	20.7041(9)	16.2000(4)
α (deg)	100.9770(10)	83.502(2)	90
β (deg)	94.8970(10)	76.853(2)	108.4080(10)
γ (deg)	94.9310(10)	73.030(2)	90
V (Å^3)	1348.02(6)	3496.8(3)	3088.65(14)
D_{calc} (g/cm^3)	1.738	1.982	2.061
$2\theta_{max}$ (deg)	54.00	52.00	56.00
R_1, wR_2 [$I > 2\sigma(I)$]	0.0239, 0.0601	0.0730, 0.1692	0.0771, 0.2288
R_1, wR_2 [all data]	0.0261, 0.0615	0.1157, 0.1990	0.0871, 0.2420
Goodness-of-fit on F^2	1.058	1.018	1.061
No. of reflection used [$>2\sigma(I)$]	5882 [R_{int} = 0.0242]	13730 [R_{int} = 0.0769]	7458 [R_{int} = 0.0449]
Refinement	full-matrix	full-matrix	full-matrix

Table S2 Selected bond lengths (Å) and bond angles (°) for **1**

Ag1-N1	2.352(1)	Ag1-N2	2.487(2)
Ag1-O1	2.896(1)	Ag1-O2	2.878(1)
Ag1-S1	2.593(2)	Ag1-S2	2.609(1)
N1-Ag1-N2	165.3(1)	N1-Ag1-O1	65.7(1)
N1-Ag1-O2	62.6(1)	N1-Ag1-S1	107.6(1)
N1-Ag1-S2	99.9(1)	N2-Ag1-O1	129.0(1)
N2-Ag1-O2	103.0(1)	N2-Ag1-S1	79.9(1)
N2-Ag1-S2	79.4(1)	O1-Ag1-O2	127.2(1)
O1-Ag1-S1	72.6(1)	O1-Ag1-S2	98.2(1)
O2-Ag1-S1	133.2(1)	O2-Ag1-S2	81.1(1)
S1-Ag1-S2	143.3(2)		

Table S3 Selected bond lengths (Å) and bond angles (°) for **2a**

Ag1-N1	2.262(7)	Ag1-N2	2.354(9)
Ag1-O1	3.029(6)	Ag1-O2	2.924(6)
Ag1-S1	2.944(2)	Ag1-S2	2.833(2)
Ag2-S2	2.423(2)	Ag2-S3	2.418(2)
Ag3-N3	2.197(7)	Ag3-N4	2.231(7)
Ag3-O3	2.942(6)	Ag3-O4	3.141(6)
Ag3-S3	2.896(2)	Ag3-S4	3.079(2)
Ag4-S4	2.419(2)	Ag4-S1A	2.411(2)
N1-Ag1-N2	164.5(3)	N1-Ag1-O1	64.5(2)
N1-Ag1-O2	66.4(2)	N1-Ag1-S1	107.5(2)
N1-Ag1-S2	108.9(2)	N2-Ag1-O1	124.8(2)
N2-Ag1-O2	103.7(2)	N2-Ag1-S1	70.6(2)
N2-Ag1-S2	76.7(2)	N3-Ag3-N4	168.8(3)
N3-Ag3-O3	62.4(2)	N3-Ag3-O4	67.4(2)
N3-Ag3-S3	106.0(2)	N3-Ag3-S4	99.9(2)
N4-Ag3-O3	123.6(2)	N4-Ag3-O4	106.6(2)
N4-Ag3-S3	78.7(2)	N4-Ag3-S4	75.1(2)
O1-Ag1-O2	130.9(2)	O1-Ag1-S1	64.9(1)
O1-Ag1-S2	125.4(1)	O2-Ag1-S1	135.7(1)
O2-Ag1-S2	69.3(1)	O3-Ag3-O4	129.7(2)
O3-Ag3-S3	68.3(1)	O3-Ag3-S4	127.1(1)
O4-Ag3-S3	129.0(1)	O4-Ag3-S4	61.4(1)
S1-Ag1-S2	142.5(1)	S2-Ag2-S3	161.6(1)
S3-Ag3-S4	153.8(1)	S4-Ag4-S1A	169.9(1)

Symmetry operations: (A) x-1, y+1, z (B) x+1, y-1, z

Table S4 Selected bond lengths (Å) and bond angles (°) for **2b**

Ag1-N1	2.296(11)	Ag1-N2	2.410(12)
Ag1-O1	2.895(11)	Ag1-O2	2.811(10)
Ag1-S1	2.787(3)	Ag1-S2	2.645(3)
Ag2-S2	2.432(3)	Ag2-S1A	2.506(3)
Ag2-F1	2.45(3)		
N1-Ag1-N2	161.9(4)	N1-Ag1-O1	66.2(4)
N1-Ag1-O2	64.7(4)	N1-Ag1-S1	104.1(3)
N1-Ag1-S2	110.9(3)	N2-Ag1-O1	127.8(3)
N2-Ag1-O2	103.9(3)	N2-Ag1-S1	76.1(3)
N2-Ag1-S2	78.8(3)	O1-Ag1-O2	128.0(3)
O1-Ag1-S1	66.1(2)	O1-Ag1-S2	103.9(2)
O2-Ag1-S1	143.0(2)	O2-Ag1-S2	78.7(2)
S1-Ag1-S2	135.5(1)	S1A-Ag2-F1	86.2(9)
S2-Ag2-S1A	140.3(1)	S2-Ag2-F1	133.3(9)

Symmetry operations: (A) x, -y+3/2, z+1/2 (B) x, -y+3/2, z-1/2

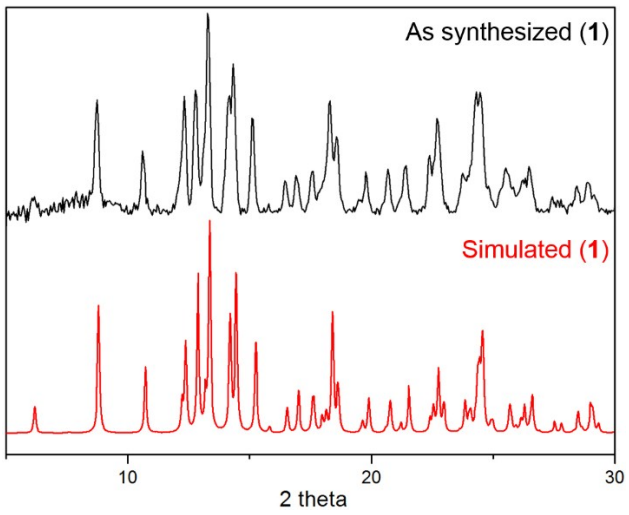

Fig. S1 PXRD patterns of **1**.

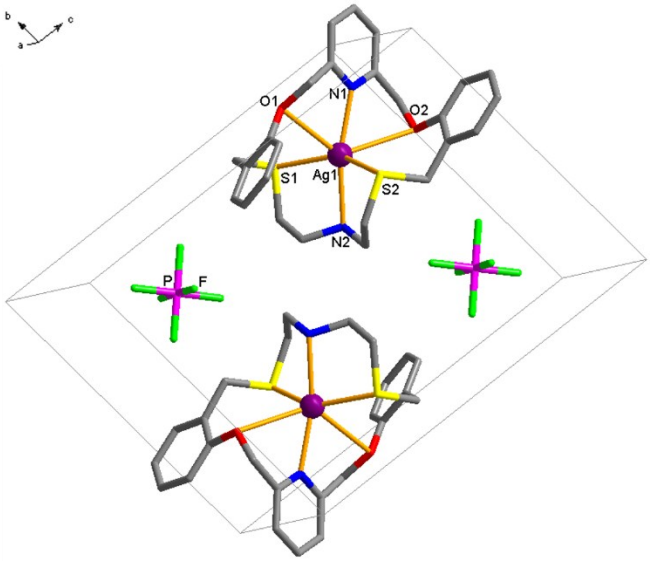

Fig. S2 Crystal structure of the silver(I) hexafluorophosphate complex **1**, [Ag(**L**)]PF_6.