Electronic Supplementary Information

For

Influence of anion and mole-ratio on the formation of 2-D coordination networks of thiacalix[4]-*bis*-monothiacrown-5

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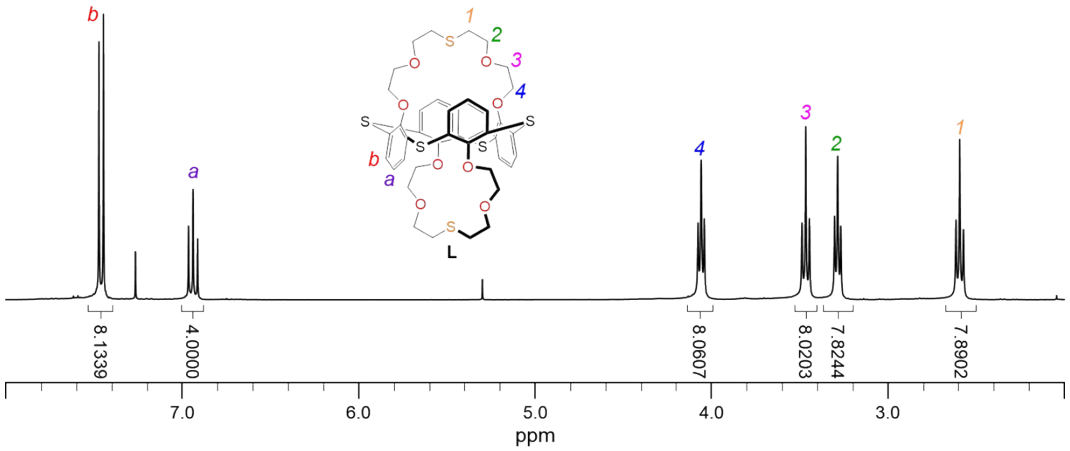
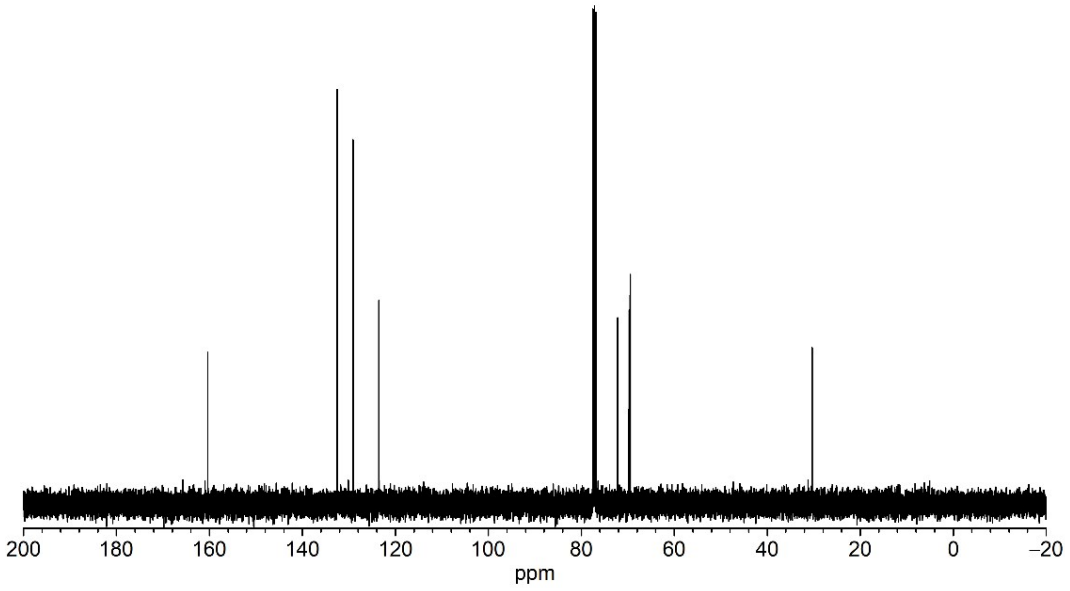


(a)



(b)

Fig. S1 (a) ^{1}H and (b) ^{13}C NMR spectra of **L** in $CDCl_3$.

Table S1 Crystal and experimental data

	1	**2**	**3**
Formula	$C_{60}H_{66}AgF_6O_{12}PS_9$	$C_{65}H_{71}AgCl_9F_3O_{15}S_9$	$C_{265}H_{273}Ag_8Cl_3F_{24}O_{65}S_{36}$
Formula weight	1520.50	1864.67	7077.29
Temperature (K)	173(2)	173(2)	173(2)
Crystal system	Trigonal	Orthorhombic	Monoclinic
Space group	*R*-3*c*	*Pbcn*	*Cc*
Z	12	8	2
a (Å)	21.9383(2)	29.7592(3)	29.0458(15)
b (Å)	21.9383(2)	26.2631(3)	26.4503(14)
c (Å)	46.0355(5)	20.0331(2)	19.6654(11)
α (°)	90	90	90
β (°)	90	90	98.978(3)
γ (°)	120	90	90
V (Å^3)	19188.0(4)	15657.2(3)	14923.2(14)
D_{calc}(g/cm^3)	1.579	1.582	1.575
μ (mm^{-1})	0.712	0.873	0.882
$2\theta_{max}$ (°)	52	52	52
Reflections Collected	63688	247090	74128
No. of reflection used	4205	15400	23286
[>2σ(*I*)]	[R_{int} = 0.0413]	[R_{int} = 0.0779]	[R_{int} = 0.01127]
Goodness-of-fit on F^2	1.053	1.050	1.007
R_1, wR_2[I > 2σ(I)]	0.0306, 0.0739	0.0678, 0.1878	0.0743, 0.1657
R_1, wR_2[all data]	0.0374, 0.0805	0.0911, 0.2117	0.1494, 0.2129

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

Ag1-S4	2.546(1)	Ag1-S4A	2.546(1)
Ag1-S4B	2.546(1)	S4-Ag1-S4A	115.02(1)
S4-Ag1-S4B	115.02(1)	S4A-Ag1-S4B	115.02(1)

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

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

Ag1-S5	2.584(1)	Ag1-S6B	2.557(2)
Ag1-S10	2.628(1)	Ag1-O13	2.376(2)
O13-Ag1-S6B	113.1(9)	O13-Ag1-S5	92.6(5)
S6B-Ag1-S5	116.5(1)	O13-Ag1-S10	122.6(8)
S6B-Ag1-S10	108.4(1)	S5-Ag1-S10	102.8(1)

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

Table S4 Selected bond lengths (Å) and bond angles (°) for **3**

Ag1-S5	2.527(5)	Ag1-S11	2.561(5)
Ag1-S17	2.620(5)	Ag1-O25	2.42(2)
Ag2-S6A	2.517(5)	Ag2-S11	2.551(5)
Ag2-O10	2.729(13)	Ag2-O27	2.40(3)
Ag3-S6A	2.461(5)	Ag3-S17	2.684(5)
Ag3-O19	2.846(12)	Ag3-O30	2.31(4)
Ag4-S12	2.497(5)	Ag4-S18B	2.528(5)
Ag4-O13	5.709(11)	Ag4-O31	2.262(16)
O25-Ag1-S5	97.2(7)	O25-Ag1-S11	107.4(6)
S5-Ag1-S11	124.32(15)	O25-Ag1-S17	119.2(7)
S5-Ag1-S17	109.85(15)	S11-Ag1-S17	100.35(15)
O27-Ag2-S6A	135.9(7)	O27-Ag2-S11	107.3(7)
S6A-Ag2-S11	116.69(16)	O27-Ag2-O10	85.0(6)
S6A-Ag2-O10	108.6(3)	S11-Ag2-O10	74.8(3)
O30-Ag3-S6A	141.1(10)	O30-Ag3-S17	104.1(9)
S6A-Ag3-S17	103.42(15)	O30-Ag3-O19	121.2(10)
S6A-Ag3-O19	93.0(3)	S17-Ag3-O19	72.8(3)
O31-Ag4-S12	138.7(4)	O31-Ag4-S18B	96.9(4)
S12-Ag4-S18B	122.84(16)	O31-Ag4-O13	80.5(4)
S12-Ag4-O13	81.22(14)	S18B-Ag4-O13	130.58(15)

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