SUPPORTING INFORMATION OF

EXOCYCLIC SELF-ASSEMBLY BEHAVIORS OF CARBOXYLIC ACID AND LARIAT ETHER MACROCYCLIC HOSTS: REGULATION BY PENDENT ARM

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Table S1: Torsion angles in the pendant arms of complexes **1**, **2, 3** and complex **4**;

Structure No.	**1**	**2**	**3**	**4**
C5–O3–C11–C12	177.93(18)	177.7(2)	-177.77(18)	-177.1(2)
O3–C11–C12–N1	-171.34(17)	-165.1(2)	169.50(18)	169.3(3)
C11–C12–N1–C13	-141.73(19)	-145.2(2)	143.7(2)	142.6(3)
C11–C12–N1–C15	89.3(2)	83.9(2)	-86.7(2)	-88.8(3)
C12–N1–C13–C14	-77.2(2)	-75.8(3)	75.8(3)	75.0(3)
N1–C13–C14–O4	53.4(3)	50.8(3)	-52.6(3)	-52.8(3)
C13–C14–O4–C6#	169.00(18)	169.5(2)	-169.38(19)	-169.8(2)

C12–N1–C15–C16	-177.12(19)	-171.6(4)	168.5(2)	177.5(2)
C14–C13–N1–C15	50.4(3)	51.9(3)	-51.5(3)	-52.2(2)
C13–N1–C15–C16	54.8(2)	59.1(4)	-63.5(3)	-54.5(3)
N1–C15–C16–C17	175.2(2)			128.9(4)
C15–C16–C17–C18	173.5(3)			
N1–C15–C16–O5		-83.6(7)	79.1(3)	
C15–C16–O5–C17		-177.7(16)	-168.0(2)	
C16–05–C17–C18			-175.6(2)	

Table S2: Torsion angles in the pendant arms of salts **5, 6** and **7**;

	5	**6**	**7**		**5**	**6**	**7**
O1A-C1A-C2A-C3A	-178.0(3)	-177.8(5)	179.6(5)	C12A-C7A-O3A-C16A	2.9(5)	-3.4(9)	-10.5(7)
O1A-C1A-C6A-C5A	178.5(3)	179.3(6)	-179.5(6)	C12A-C7A-C8A-O4A	179.3(3)	-179.5(5)	-177.9(4)
C6A-C1A-O1A-C13A	4.2(5)	-4.0(9)	0.0(8)	C8A-C7A-C12A-C11A	-2.5(6)	0.5(9)	-0.6(8)
C6A-C1A-C2A-O5A	-178.3(3)	-177.9(5)	-178.8(5)	O4A-C8A-C9A-C10A	-177.6(4)	178.4(6)	178.4(5)
C2A-C1A-C6A-C5A	-2.3(5)	0.1(9)	0.1(10)	C9A-C10A-C11A-C12A	-0.8(8)	-1.5(10)	1.8(9)
O1A-C1A-C2A-O5A	1.0(4)	2.8(8)	0.8(8)	O1A-C13A-C14A-O2A	-60.8(4)	-66.7(6)	-72.1(6)
C6A-C1A-C2A-C3A	2.7(5)	1.5(9)	0.0(9)	O2A-C15A-C16A-O3A	70.9(4)	71.5(6)	63.4(6)
C1A-C2A-O5A-C20A	169.6(3)	175.9(5)	174.0(5)	O4A-C17A-C18A-N1A	-61.0(4)	-66.5(6)	52.0(5)
C3A-C2A-O5A-C20A	-11.5(5)	-3.5(9)	-4.8(8)	C20A-C19A-N1A-C18A	-174.0(3)	-180.0(4)	58.6(6)
C2A-C3A-C4A-C5A	-0.1(5)	-0.1(9)	1.0(12)	C19A-C20A-O5A-C2A	-174.3(3)	-172.9(5)	-175.8(4)
C8A-C7A-O3A-C16A	-176.6(3)	177.4(5)	170.2(4)	C1A-C2A-C3A-C4A	-1.5(5)	-1.5(9)	-0.6(10)
O3A-C7A-C8A-C9A	-179.3(3)	178.7(5)	-178.8(4)	C4A-C5A-C6A-C1A	0.7(6)	-1.7(9)	0.4(12)
O3A-C7A-C12A-C11A	178.0(4)	-178.7(6)	-179.9(5)	O3A-C7A-C8A-O4A	-1.1(4)	-0.3(8)	1.4(6)
C9A-C8A-O4A-C17A	3.4(5)	4.5(9)	-9.3(7)	C12A-C7A-C8A-C9A	1.2(5)	-0.6(9)	1.9(7)
C8A-C9A-C10A-C11A	-0.6(7)	1.4(9)	-0.5(8)	C7A-C8A-O4A-C17A	-174.7(3)	-176.7(5)	170.5(4)
C14A-C13A-O1A-C1A	-177.6(3)	-168.6(5)	175.1(5)	C7A-C8A-C9A-C10A	0.4(6)	-0.3(9)	-1.4(8)
C16A-C15A-O2A-C14A	-175.7(3)	173.9(5)	-178.1(5)	C10A-C11A-C12A-C7A	2.3(7)	0.6(9)	-1.3(8)
C18A-C17A-O4A-C8A	176.1(3)	-175.2(5)	-178.6(4)	C13A-C14A-O2A-C15A	178.7(3)	174.8(5)	168.8(5)
C17A-C18A-N1A-C21A	-167.0(3)	-63.8(6)	44.5(6)	C15A-C16A-O3A-C7A	-175.6(3)	176.1(5)	177.9(4)
N1A-C19A-C20A-O5A	-55.1(4)	62.7(6)	58.7(6)	C17A-C18A-N1A-C19A	-41.0(4)	171.1(4)	173.4(4)
C22A-C21A-N1A-C19A	175.1(7)	-97.7(5)	-65.4(5)	C20A-C19A-N1A-C21A	-48.5(4)	55.3(6)	-171.3(4)

O5A-C2A-C3A-C4A	179.6(3)	177.8(6)	178.2(7)	C22A-C21A-N1A-C18A	-58.6(8)	140.0(4)	64.0(5)
C21A-C22A-C23A-C24A	62.4(13)		-178.5(5)				
N1A-C21A-C22A-C23A	177.3(7)		-176.9(4)				
C22A-C23A-C24A-C25A			179.7(5)				
C21A-C22A-O6A-C23A		167.2(5)					
C23A-C24A-C25A-C26A		-172.3(7)					
C24A-C23A-O6A-C22A		-176.3(5)					
O6A-C23A-C24A-C25A		-64.6(8)					

Table S3: Hydrogen bonds for complex **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(1)	0.871(19)	1.77(2)	2.631(2)	172(5)
C(11)-H(11A)...O(2)#3	0.99	2.40	3.373(3)	168.8
C(13)-H(13A)...O(2)	0.99	2.56	3.311(3)	132.4
C(15)-H(15B)...O(2)#3	0.99	2.47	3.458(3)	172.3
C(16)-H(16D)...O(2)	0.99	2.63	3.407(3)	135.7
C(13)-H(13B)...O(3)#4	0.99	2.62	3.490(3)	146.8
C(12)-H(12B)...O(4)#5	0.99	2.64	3.558(3)	154.3

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 -x+1/2,-y+3/2,-z+1 #3 x,y+1,z

#4 x,y-1,z #5 -x+1/2,-y+1/2,-z+1

Table S4: Hydrogen bonds for complex **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...N(1)	0.87(2)	1.74(2)	2.584(3)	164(5)
O(6)-H(6A)...O(2)	0.86	2.16	2.987(8)	161.9
C(13)-H(13A)...O(2)	0.99	2.46	3.198(3)	131.3
C(17)-H(17C)...O(6)	0.98	2.64	3.62(2)	175.4
C(14)-H(14B)...O(5)	0.99	2.44	3.180(6)	131.2
C(11)-H(11A)...O(2)#3	0.99	2.57	3.549(3)	170.7
C(15)-H(15B)...O(2)#3	0.99	2.40	3.352(3)	160.5
C(12)-H(12B)...O(4)#4	0.99	2.62	3.584(3)	164.0
C(13)-H(13B)...O(3)#5	0.99	2.70	3.646(3)	159.7

C(16)-H(16B)...O(6)#3	0.99	2.32	3.178(18)	144.2

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+2 #2 -x+1/2,-y+5/2,-z+2 #3 x,y+1,z

#4 -x+1/2,-y+3/2,-z+2 #5 x,y-1,z

Table S5: Hydrogen bonds for complex **3** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1B)...N(1)	0.90(6)	1.71(6)	2.611(3)	176(5)
C(13)-H(13A)...O(2)	0.99	2.49	3.245(3)	133.2
C(16)-H(16A)...O(2)	0.99	2.58	3.379(3)	137.9
C(14)-H(14B)...O(5)	0.99	2.47	3.150(3)	125.8
C(11)-H(11A)...O(2)#3	0.99	2.48	3.456(3)	168.8
C(15)-H(15B)...O(2)#3	0.99	2.36	3.312(3)	161.3
C(12)-H(12B)...O(4)#4	0.99	2.61	3.541(3)	156.9
C(13)-H(13B)...O(3)#5	0.99	2.64	3.550(3)	152.2
C(9)-H(9)...O(5)#6	0.95	2.62	3.478(3)	150.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2 #2 -x+2,-y,-z+1 #3 x+1,y,z

#4 -x+1,-y,-z+1 #5 x-1,y,z #6 x+1,y+1,z

Table S6: Hydrogen bonds for complex **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(1)	0.87(4)	1.75(4)	2.621(3)	177(4)
C(13)-H(13A)...O(2)	0.99	2.54	3.263(4)	129.9
C(16)-H(16)...O(2)	0.95	2.80	3.518(4)	133.5
C(11)-H(11A)...O(2)#3	0.99	2.41	3.391(4)	170.4
C(15)-H(15B)...O(2)#3	0.99	2.56	3.543(4)	169.9
C(12)-H(12B)...O(4)#4	0.99	2.66	3.600(4)	157.8
C(13)-H(13B)...O(3)#5	0.99	2.62	3.536(4)	153.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z #2 -x+1/2,-y+1/2,-z #3 x,y-1,z

#4 -x+1/2,-y+3/2,-z #5 x,y+1,z

Table S7. Hydrogen bonds for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

Water in the cavity of the crown – crown ether				
N(1A)-H(1A)...O(10)#1	0.879(18)	1.890(19)	2.763(4)	172(3)
N(1B)-H(1B)...O(15)	0.890(16)	1.804(17)	2.689(4)	173(3)
N(1C)-H(1C)...O(11)	0.898(17)	1.848(18)	2.736(3)	169(3)
O(10)-H(10D)...O(1A)#1	0.841(17)	2.174(17)	3.008(3)	171(3)
O(10)-H(10D)...O(1A)#1	0.841(17)	2.174(17)	3.008(3)	171(3)
O(10)-H(10D)...O(2A)#1	0.841(17)	2.67(3)	3.066(3)	110(3)
O(10)-H(10C)...O(3A)#1	0.831(17)	2.14(2)	2.958(3)	167(3)
O(10)-H(10C)...O(4A)#1	0.831(17)	2.46(3)	2.985(3)	122(3)
O(10)-H(10D)...O(5A)#1	0.841(17)	2.53(3)	3.042(4)	120(3)
O(11)-H(11D)...O(1C)	0.831(16)	2.124(18)	2.938(3)	167(3)
O(11)-H(11C)...O(2C)	0.837(16)	2.71(3)	3.080(3)	108(2)
O(11)-H(11C)...O(3C)	0.837(16)	2.085(17)	2.915(3)	171(3)
O(11)-H(11C)...O(4C)	0.837(16)	2.50(3)	2.978(3)	117(3)
O(11)-H(11D)...O(5C)	0.831(16)	2.43(3)	2.971(4)	124(3)
O(15)-H(15D)...O(1B)	0.829(16)	2.149(17)	2.959(3)	166(3)
O(15)-H(15D)...O(2B)	0.829(16)	2.55(3)	2.948(3)	110(2)
O(15)-H(15C)...O(3B)	0.849(17)	2.061(17)	2.902(3)	171(2)
O(15)-H(15C)...O(4B)	0.849(17)	2.47(2)	2.981(3)	120(2)
O(15)-H(15D)...O(5B)	0.829(16)	2.55(3)	3.048(3)	120(3)
Interactions in the hydrated anion layer				
O(12)-H(12C)...O(14)#2	0.828(16)	1.940(17)	2.767(3)	177(4)
O(13)-H(13C)...O(19)	0.815(17)	1.826(17)	2.637(4)	173(3)
O(14)-H(14D)...O(18)	0.830(16)	1.940(19)	2.728(4)	158(3)
O(17)-H(17C)...O(16)	0.820(18)	1.832(19)	2.650(4)	177(4)
O(12)-H(12D)...O(7C)	0.846(17)	1.898(19)	2.735(3)	170(3)
O(13)-H(13D)...O(6C)#3	0.802(16)	1.975(16)	2.771(3)	171(3)
O(14)-H(14C)...O(7C)#4	0.838(17)	2.014(19)	2.839(3)	168(3)
O(16)-H(16C)...O(8B)	0.847(17)	1.909(18)	2.736(4)	165(3)
O(16)-H(16D)...O(8B)#5	0.862(17)	2.53(3)	3.090(3)	124(3)
O(16)-H(16D)...O(9B)#5	0.862(17)	1.953(17)	2.813(3)	175(3)
O(17)-H(17D)...O(6A)#6	0.827(18)	1.87(2)	2.673(4)	163(4)
O(18)-H(18C)...O(6C)#4	0.854(17)	1.945(18)	2.788(4)	169(3)
O(18)-H(18D)...O(7A)#7	0.855(18)	1.80(2)	2.638(5)	168(5)
O(19)-H(19C)...O(9B)#5	0.811(18)	1.96(2)	2.774(4)	176(5)
O(19)-H(19D)...O(6A)#6	0.812(18)	2.13(2)	2.935(4)	173(5)
O(19)-H(19D)...O(7A)#6	0.812(18)	2.50(3)	3.083(4)	129(4)
O(9A)-H(9AB)...O(17)	0.828(18)	1.741(19)	2.559(3)	169(4)
O(7B)-H(7BA)...O(12)	0.833(18)	1.82(2)	2.631(4)	164(4)
O(8C)-H(8CA)...O(13)#5	0.850(18)	1.729(19)	2.576(3)	174(4)
Hydrogen bond between crown ether and acid anions				
C(3A)-H(3AA)...O(8B)	0.95	2.52	3.464(4)	173.3
C(9A)-H(9AA)...O(8A)#5	0.95	2.64	3.585(5)	170.5

C(14B)-H(14A)...O(8C)	0.99	2.56	3.481(4)	155.1	
C(19B)-H(19A)...O(6C)#7	0.99	2.64	3.351(4)	128.5	
C(19B)-H(19A)...O(7C)#7	0.99	2.43	3.299(4)	146.5	
C(21A)-H(21G)...O(6A)#8	0.99	2.61	3.470(5)	145.4	
C(21D)-H(21I)...O(6A)#8	0.99	2.53	3.470(5)	158.7	
Hydrogen bond between crown ether and water in hydrated anion layer					
C(17B)-H(17B)...O(18)#9	0.99	2.59	3.577(5)	173.0	

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 x-1,y,z #3 x,y,z+1 #4 -x+1,-y+1,-z

#5 -x+1,-y,-z+1 #6 -x,-y+1,-z+1 #7 x+1,y,z

#8 x+1,y-1,z #9 -x+2,-y+1,-z

Table S8 Hydrogen bonds for **6** [Å and °].

Donor--H..Acceptor	[ARU]	D - H	H...A	H...A	D - H...A
Hydrogen bond in cation sheet					
N1A--H1A..O5A	[ ]	0.88(4)	2.57(6)	2.917(5)	104(3)
N1A--H1A..O6A	[ ]	0.88(4)	2.46(6)	2.873(6)	109(5)'
N1A--H1A..O7A	[1556.05]	0.88(3)	1.92(4)	2.699(6)	146(6)"
N1B--H1B..O5B	[ ]	0.88(3)	2.59(6)	2.948(5)	106(3)
N1B--H1B..O6B	[ ]	0.88(3)	2.50(4)	2.894(6	108(4)'
N1B--H1B..O7B	[1555.06]	0.88(3)	1.89(4)	2.674(6)	148(4)"
O7A--H7AA..O1A	[1554.01]	0.83(3)	2.19(3)	3.016(5)	175(7)
O7A--H7AA..O2A	[1554.01]	0.83(3)	2.57(7)	2.993(6)	113(5)'
O7A--H7AA..O5A	[1554.01]	0.83(3)	2.49(7)	2.864(5)	108(6)"
O7A--H7AB..O3A	[1554.01]	0.80(5)	2.14(5)	2.920(6)	163(5)
O7A--H7AB..O4A	[1554.01]	0.80(5)	2.34(4)	2.858(5)	123(4)'
O7B--H7BA..O3B	[1555.02]	0.81(5)	2.07(4)	2.876(5)	170(6)
O7B--H7BA..O4B	[1555.02]	0.81(5)	2.42(4)	2.869(5)	116(4)'
O7B--H7BB..O1B	[1555.02]	0.80(4)	2.23(3)	3.013(5)	167(5)
O7B--H7BB..O5B	[1555.02]	0.80(4)	2.34(4)	2.808(5)	118(4)'
Hydrogen bond in anion layer (acid-acid)					
O11A--H11C..O8A	[4755.03]	0.83(3)	1.70(3)	2.510(5)	166(7)
O11B--H11D..O8B	[4655.04]	.85	1.61	2.450(5)	172
O11B--H11D..O9B	[4655.04]	0.85	2.5	3.083(6)	127'
Hydrogen bond in anion layer (water-acid)					
O12--H12F..O8A	[1455.03]	0.84(4)	1.98(4)	2.806(7)	170(4)
O13--H13E..O9A	[1555.03]	0.86(4)	1.91(5)	2.752(7)	166(7)
O13--H13F..O9B	[1555.04]	0.83(3)	1.95(3)	2.716(7)	153(6)
O14--H14F ..O11B	[4645.04]	0.84(4)	2.06(3)	2.878(8)	168(8)
O15--H15E ..O10A	[1555.03]	0.84(6)	2.23(6)	2.920(8)	140(5)
O15--H15E..O10B	[1555.04]	0.84(6)	2.59(6)	3.081(7)	119(5)'
O15--H15F..O8B	[4655.04]	0.84(4)	2.01(3)	2.847(8)	174(10)

O16--H16E..O14	[1555.09]	0.85(6)	1.91(6)	2.708(8)	158(5)
O16--H16F..O12	[4645.07]	0.84(4)	2.02(6)	2.787(7)	152(6)
O17--H17E..O16	[1555.11]	0.85(7)	2.18(8)	2.934(9)	149(9)
O17--H17F..O13	[1555.08]	0.83(8)	1.98(8)	2.799(10)	170(7)
Weak Hydrogen bond between ion pairs					
C15B--H15D..O9B	[4656.04]	0.99	2.56	3.396(9)	142
C18A--H18A..O16	[2655.11]	0.99	2.34	3.206(8)	146
C20A--H20A..O10B	[2665.04]	0.99	2.47	3.263(7)	136
C20A--H20B..O10A	[2665.03]	0.99	2.53	3.456(7)	157
C29A--H29B..O10B	[1555.04]	0.95	2.56	3.494(8)	169
intraC22B--H22D..O5B	[ ]	0.99	2.54	3.341(7)	138
intraC28A--H28B..O9A	[ ]	0.95	2.4	2.734(7)	100

Translation of ARU-Code to CIF and Equivalent Position Code

[1556.] = [1_556] =x,y,1+z

[2665.] = [2_665] =3/2-x,1-y,1/2+z

[2655.] = [2_655] =3/2-x,-y,1/2+z

[4656.] = [3_656] =1-x,1/2+y,3/2-z

[1554.] = [1_554] =x,y,-1+z

[4755.] = [3_755] =2-x,1/2+y,1/2-z

[4645.] = [3_645] =1-x,-1/2+y,1/2-z

[4655.] = [3_655] =1-x,1/2+y,1/2-z

[1455.] = [1_455] =-1+x,y,z

Table S9 Hydrogen bonds for **7** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
Water in the cavity of the crown – crown ether				
N(1A)-H(1A)...O(6A)	0.873(19)	1.84(2)	2.682(5)	162(4)
N(1B)-H(1B)...O(6B)	0.868(19)	1.84(3)	2.662(5)	158(4)
N(1C)-H(1C)...O(6C)#2	0.868(18)	1.84(2)	2.672(5)	160(4)
O(6A)-H(6AB)...O(1A)	0.827(18)	2.06(2)	2.868(5)	166(5)
O(6A)-H(6AB)...O(2A)	0.827(18)	2.65(5)	2.954(5)	103(4)
O(6A)-H(6AC)...O(3A)	0.797(19)	2.05(2)	2.832(5)	169(5)
O(6A)-H(6AC)...O(4A)	0.797(19)	2.56(4)	3.040(5)	120(4)
O(6A)-H(6AB)...O(5A)	0.827(18)	2.49(4)	2.943(5)	116(4)
O(6B)-H(6BB)...O(1B)	0.811(18)	2.07(2)	2.863(5)	168(5)
O(6B)-H(6BB)...O(2B)	0.811(18)	2.69(5)	3.012(5)	106(4)
O(6B)-H(6BC)...O(3B)	0.823(19)	2.03(2)	2.822(5)	163(5)
O(6B)-H(6BC)...O(4B)	0.823(19)	2.44(4)	3.001(5)	126(4)
O(6B)-H(6BB)...O(5B)	0.811(18)	2.49(4)	2.910(5)	114(4)
O(6C)-H(6CC)...O(1C)#3	0.812(18)	1.996(19)	2.797(5)	168(3)

O(6C)-H(6CB)...O(2C)#3	0.816(18)	2.69(5)	2.975(5)	102(4)
O(6C)-H(6CB)...O(3C)#3	0.816(18)	2.08(2)	2.879(5)	168(5)
O(6C)-H(6CB)...O(4C)#3	0.816(18)	2.43(4)	2.891(5)	117(4)
O(6C)-H(6CC)...O(5C)#3	0.812(18)	2.52(3)	3.023(5)	121(3)
Interactions in the hydrated anion layer				
O(13)-H(13G)...O(20)	0.844(19)	1.98(3)	2.775(6)	157(5)
O(16)-H(16G)...O(17)	0.816(18)	2.02(2)	2.795(6)	159(4)
O(18)-H(18G)...O(19)	0.824(19)	1.98(3)	2.737(5)	153(5)
O(19)-H(19G)...O(16)#4	0.835(19)	1.95(2)	2.762(5)	165(6)
O(20)-H(20G)...O(18)	0.832(19)	1.91(2)	2.700(6)	158(5)
O(20)-H(20H)...O(14)	0.836(19)	1.89(2)	2.712(6)	167(5)
O(21)-H(21G)...O(22)#5	0.825(19)	1.99(2)	2.804(6)	168(6)
O(21)-H(21H)...O(26)#5	0.826(19)	1.973(19)	2.792(6)	171(5)
O(22)-H(22G)...O(13)	0.849(19)	2.05(3)	2.870(6)	163(5)
O(22)-H(22H)...O(25)	0.849(19)	1.99(3)	2.755(8)	150(6)
O(25)-H(25G)...O(27)	0.84(2)	1.90(4)	2.702(7)	159(9)
O(25)-H(25H)...O(15)	0.83(2)	1.96(2)	2.788(7)	173(6)
O(27)-H(27G)...O(24)	0.85	1.77	2.621(7)	178.2
O(23)-H(23K)...O(21)#5	0.85	1.91	2.760(9)	178.8
O(23)-H(23L)...O(29)#6	0.85	1.93	2.777(11)	178.6
O(13)-H(13H)...O(7)	0.821(19)	2.05(3)	2.850(6)	163(5)
O(14)-H(14G)...O(7)	0.830(19)	1.90(2)	2.702(5)	163(5)
O(14)-H(14H)...O(11)	0.829(19)	1.91(3)	2.710(5)	161(5)
O(15)-H(15G)...O(9)#4	0.826(19)	1.99(2)	2.810(6)	173(6)
O(16)-H(16H)...O(12)	0.811(19)	2.05(3)	2.823(5)	159(5)
O(17)-H(17G)...O(8)	0.841(19)	1.899(19)	2.723(6)	166(5)
O(17)-H(17H)...O(11)	0.847(19)	1.90(2)	2.733(5)	169(5)
O(19)-H(19H)...O(12)#1	0.824(19)	1.92(2)	2.739(5)	170(5)
O(24)-H(24G)...O(8)#4	0.83(2)	1.97(2)	2.791(7)	174(7)
O(26)-H(26G)...O(10)	0.85	1.87	2.723(7)	177.8
O(28)-H(28D)...O(9)	0.85	1.84	2.683(11)	171.5
O(28)-H(28D)...O(9)	0.85	1.84	2.683(11)	171.5
O(29)-H(29G)...O(10)	0.85	1.93	2.762(8)	164.9
Water in anion layer... crown				
O(18)-H(18H)...O(2A)#4	0.806(19)	2.12(2)	2.918(5)	170(6)
O(24)-H(24H)...O(2B)#2	0.834(19)	2.35(4)	3.067(6)	145(6)
O(29)-H(29H)...O(2C)#7	0.85	2.18	3.009(7)	165.3
Crown ... water in anion layer				
C(3C)-H(3CA)...O(29)#5	0.95	2.65	3.593(8)	171.1
C(13A)-H(13B)...O(16)	0.99	2.65	3.373(7)	130.5
C(19A)-H(19A)...O(14)#3	0.99	2.43	3.332(6)	150.9
C(13B)-H(13D)...O(27)#3	0.99	2.39	3.358(8)	166.7
C(16B)-H(16C)...O(17)#8	0.99	2.53	3.480(7)	160.7
C(13C)-H(13F)...O(29)#9	0.99	2.55	3.356(8)	138.7

C(15C)-H(15F)...O(29)#1	0.99	2.41	3.343(8)	156.9	
C(16C)-H(16E)...O(26)#9	0.99	2.45	3.408(7)	161.5	
C(17C)-H(17F)...O(15)#10	0.99	2.55	3.529(7)	171.0	
C(20C)-H(20E)...O(29)#5	0.99	2.50	3.171(7)	124.4	
Crown ... acid					
C(18B)-H(18C)...O(7)	0.99	2.63	3.546(6)	154.4	
C(20A)-H(20B)...O(11)#3	0.99	2.57	3.473(6)	150.9	
Crown ... crown					
C(19A)-H(19B)...O(5B)	0.99	2.54	3.501(6)	164.6	
C(21A)-H(21A)...O(4A)	0.99	2.57	3.155(6)	118.0	
C(19B)-H(19D)...O(5A)	0.99	2.61	3.567(6)	161.9	
Intra C(21B)-H(21D)...O(4B)	0.99	2.61	3.187(6)	116.9	
C(18C)-H(18F)...O(3C)#11	0.99	2.49	3.281(6)	136.8	
C(18C)-H(18F)...O(4C)#11	0.99	2.65	3.605(6)	162.5	
Intra C(21C)-H(21E)...O(5C)	0.99	2.59	3.155(6)	116.4	

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 x-1,y,z #3 x+1,y,z #4 x,y-1,z

#5 -x+1,-y+1,-z+1 #6 -x+1,-y+1,-z #7 x+1,y,z-1

#8 x+1,y-1,z #9 x-1,y,z+1 #10 x,y,z+1 #11 -x,-y,-z+2

Table S10a: The C-H···π hydrogen bonds for complexes **1**, **2**, **3**, **4**, **5**, **6** and **7**.

C-H...π		H..Cg	H-Perp	X-H..Cg	X..Cg	X-H,Pi
Complex **I**	C7-H7B...Cg(crown)	2.65	2.64	140	3.468(3)	49
Complex **III**	C10-H19B...Cg(crown)	2.79	2.785	138	3.576	48
Complex **1**	C(7)-H(7)...Cg(crown)	2.93	2.85	146	3.751(3)	63
	C(18)-H(18D)...Cg(PTA)	3.2388(3)	3.0779	119.345(224)	3.8154(39)	
Complex **2**	C(7)-H(7)...Cg(crown)	2.81	2.77	144	3.626(3)	59
	C(17)-H(17A)...Cg(PTA)	2.87	2.83	126	3.532(9)	28
Complex **3**	C(18)-H(18C)...Cg(crown)	3.114	3.0905	133.055(180)	3.8500	
Complex **4**	C(7)-H(7)...Cg(crown)	2.73	2.69	144	3.542(3)	61
	C(17)-H(17B)...Cg(PTA)	3.2708(6)	2.8207(41)	145.099	4.0863(38)	
Complex **5**	C13C-H13G...Cg(crown)	2.50	2.49	164	3.462(4)	78
	C16B-H16B...Cg(crown)	2.71	2.60	154	3.652(3)	65
	C18B-H18A...Cg(crown)	2.65	2.64	152	3.552(3)	59
	C19C-H19G...Cg(crown)	2.71	2.69	158	3.649(4)	63
	C24B-H24A...Cg(crown)	2.98	2.95	137	3.756(9)	43

	C24C-H24G...Cg(crown)	2.85	2.83	151	3.739(5)	61
Complex **6**	C3B-H3BA...Cg(PTA)	2.71	2.69	148	3.551(6)	64
	C11B-H11B...Cg(PTA)	2.88	2.86	141	3.664(8)	58
	C18A-H18B...Cg(crown)	2.59	2.56	144	3.442(6)	57
	C18B-H18C...Cg(crown)	2.76	2.70	142	3.592(7)	59
Complex **7**	C5A-H5AA...Cg(crown)	2.96	2.61	150	3.809(8)	67
	C5B-H5BA...Cg(crown)	2.63	2.57	162	3.540(7)	68
	C11C-H11C...Cg(crown)	2.96	2.67	154	3.839(10)	57
	C23A-H23A...Cg(crown)	2.86	2.75	156	3.782(6)	63

Table S10b:the π···π interactions for complexes **3**, **5** and **7**.

π···π	Cg(I)	Res(I) Cg(J)	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
complex **3**	Cg(1)	[1] -> Cg(1)	4.1220(15)	0	30.4	30.4	-3.5567(10)	-3.5566(10)	2.084
Complex **5**	Cg(3)	[2] -> Cg(3)	4.573(2)	0.02(19)	37.1	37.1	-3.6462(16)	-3.6462(16)	2.760
Complex **7**	Cg(5)	[3] -> Cg(5)	4.492(3)	0.0(3)	43.9	43.9	3.239(2)	3.238(2)	3.113

Table S11: TGA and DSC for complex **2**.

The TG and DSC analyses of complex **2** have been performed under nitrogen atmosphere with a heating rate of 10 °C min^{-1}. The TGA measurement of **2** shows a weight loss of 0.60% in the temperature range 175-190°C, which corresponds to the loss of lattice water molecules (theoretical value of 0.56%). And the TGA measurement of **2** shows a weight loss of 0.13% in the temperature range 80-110°C, which corresponds to the loss of solvent on crystal surface.

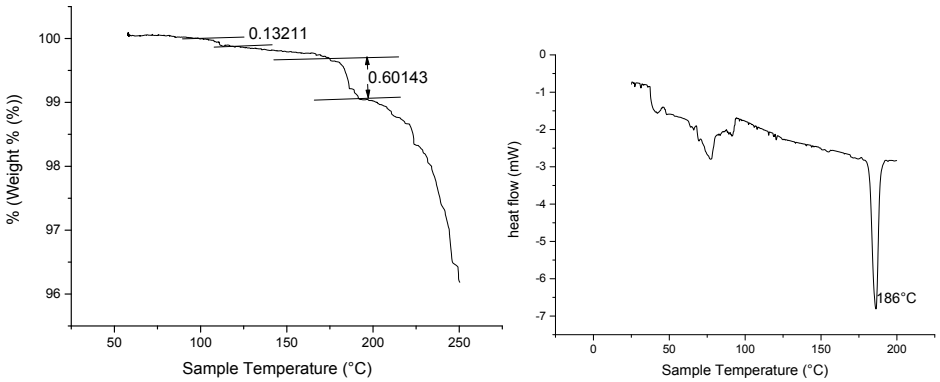

Table.s12: figure S1: FT-IR for compound **II** and complexes **1, 2, 3**, 4. Figure S2: FT-IR for PTA and complexes **1, 2, 3**.

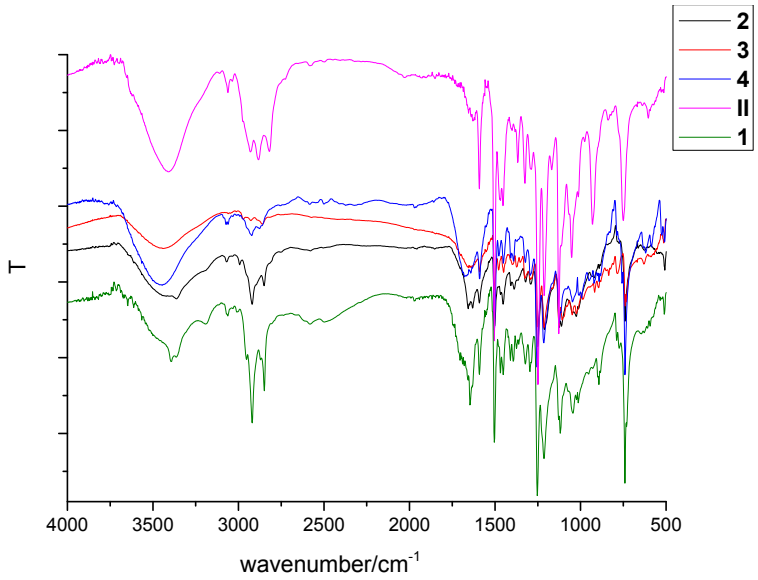

Figure s1

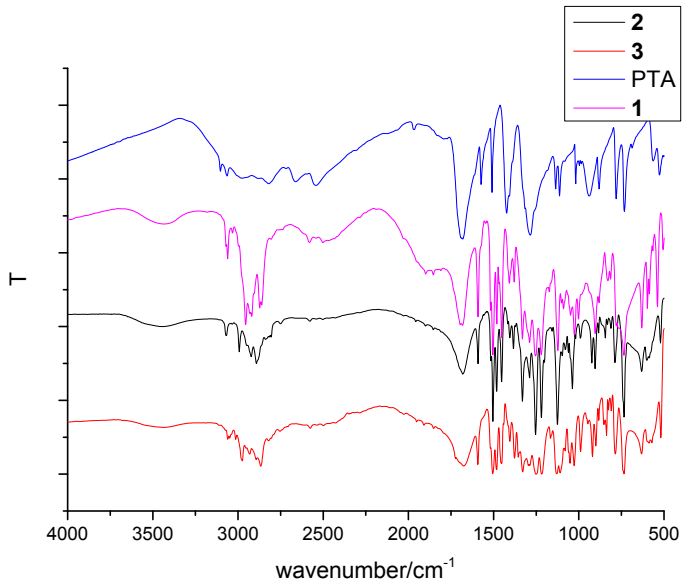

Figure s2