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Electronic Supplementary Information (ESI)

Ion-Pair Induced Self-Assembly of Molecular Barrels with Encapsulated Tetraalkylammonium Cations Based on a Bis-trisurea Stave

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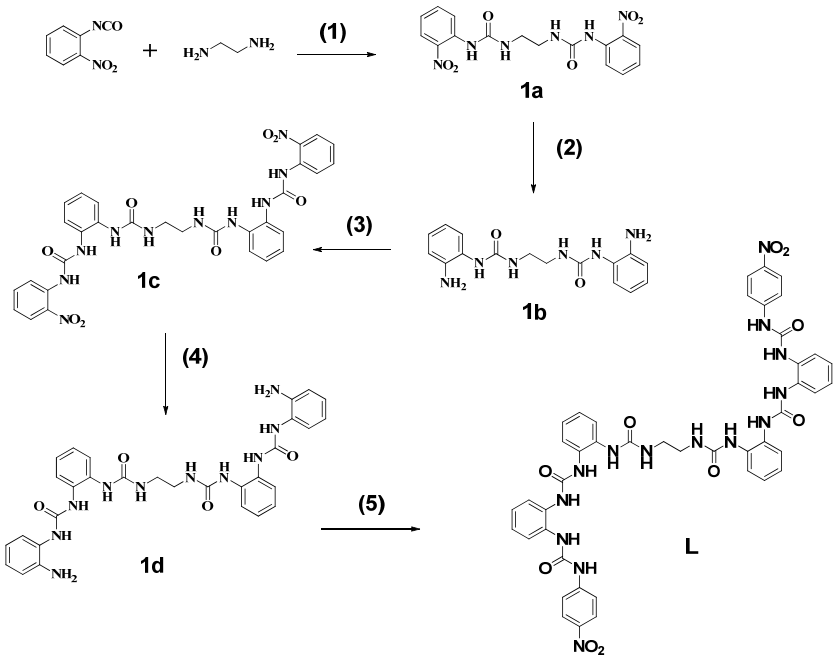
Experimental details

S1. General

The *o*-nitrophenylisocyanate and *p*-nitrophenylisocyanate were purchased from Alfa Aesar and used as received. All solvents and other reagents were of reagent grade quality. ^{1}H and ^{13}C NMR spectra were recorded on a Mercury plus-400 spectrometer at 400 MHz and 100 MHz, respectively, using TMS as an

internal standard. UV-vis spectra were performed on an HP8453 spectrophotometer (1 cm quartz cell). Elemental analyses were performed on an Elementar VarioEL instrument. IR spectra were recorded on a Bruker IFS 120HR spectrometer. ESI-MS measurements were carried out using a Waters ZQ4000 spectrometer. Melting points were detected on an X-4 Digital Vision MP Instrument.

S2. Synthesis of L



Scheme S1. Synthesis of **L**: (1) Toluene; (2) $NH_2NH_2{\cdot}H_2O$, Pd/C 10% cat., MeOH; (3) *o*-nitrophenylisocyanate, THF; (4) $NH_2NH_2{\cdot}H_2O$, Pd/C 10% cat., MeOH; (5) *p*-nitrophenylisocyanate, THF/DMSO (v/v, 5/1).

1,1'-(Ethane-1,2-diyl)bis(3-(2-nitrophenyl)urea) (1a)

A solution of ethane-1,2-diamine (0.66 g, 11.0 mmol) in 30 mL toluene was added dropwise to the *o*-nitrophenylisocyanate (4.00 g, 24.4 mmol) toluene solution (100 mL). After refluxing under stirring for 4 hours, the precipitate was filtered off and washed several times with cold THF and diethyl ether and then dried in vacuum to yield **1a** as a yellow solid (3.82 g, 90 %). M.p.: 260 °C. ^{1}H NMR (400 MHz, DMSO-d_6, ppm): δ9.42 (s, 2H, Hb), 8.33 (d, J = 8.4 Hz, 2H, H6), 8.06 (d, J = 8.4 Hz, 2H, H3), 7.67 (s, 2H, Ha), 7.63 (d, J = 7.6 Hz, 2H, H4), 7.13 (t, J = 7.6 Hz, 2H, H5), 3.14 (t, J = 2.8, 4H, CH2). ^{13}C NMR (100 MHz, DMSO-d_6), 154.3 (CO), 136.7 (C), 135.8 (CH), 134.9 (CH), 125.2 (C), 121.9 (CH), 121.4 (CH), 39.5 (CH2). IR (KBr, ν/cm^{-1}): 3339, 3093, 1655, 1566, 1503, 1341, 1264. Anal. Calcd for $C_{16}H_{16}N_6O_6$: C, 49.49; H, 4.15; N, 21.64%. Found: C, 49.44; H, 4.08; N, 21.25%. ESI-MS: *m/z* 100%, 389.0 $[M + H]^+$; 90%, 411.2 $[M + Na]^+$; 15%, 427.1 $[M + K]^+$.

1,1'-(Ethane-1,2-diyl)bis(3-(2-aminophenyl)urea) (1b)

Hydrazine monohydrate (4.0 mL) was added dropwise to the suspension of 1,1'-(ethane-1,2-diyl)bis(3-(2-nitrophenyl)urea) (**1a**, 3.00 g, 7.7 mmol) and Pd/C 10% (0.15 g, cat.) in methanol (250 mL). After refluxing for 12 hours, the solid was filtered off, dissolved in DMF (30 mL), and filtered through Celite to remove Pd/C. The DMF solution was poured in water (300 mL) and the precipitate thus obtained was filtered off, washed several times with ethanol and diethyl ether and then dried over vacuum to give **1b** as a white solid (2.07 g, 70 %). M.p.: 163 °C. ^{1}H NMR (400 MHz, DMSO-d_6, ppm): δ 7.61 (s, 2H, Hb), 7.24 (d, J = 7.2 Hz, 2H, H6), 6.79 (t, J = 7.2 Hz, 2H, H4), 6.69 (d, J = 6.8 Hz, 2H, H3), 6.54 (t, J = 6.8 Hz, 2H, H5), 6.24 (s, 2H, Ha), 4.72 (s, 4H, Hc), 3.16 (t, J = 2.8, 4H, CH2). ^{13}C NMR (100 MHz, DMSO-d_6), 156.1 (CO), 140.8 (C), 125.3 (CH), 124.0 (CH), 123.7 (C), 116.6 (CH), 115.7 (CH), 39.5 (CH_2). IR (KBr, ν/cm^{-1}): 3342, 3295, 3111, 1615, 1565, 1510, 1482, 1268. Anal. Calcd for $C_{16}H_{20}N_6O_2$: C, 58.52; H, 6.14; N, 25.59%. Found: C, 58.82; H, 5.98; N, 25.45%. ESI-MS: *m/z* 100%, 329.2 $[M + H]^+$.

1,1'-(Ethane-1,2-diyl)bis(3-(2-(3-(2-nitrophenyl)ureido)phenyl)urea) (1c)

1,1'-(Ethane-1,2-diyl)bis(3-(2-aminophenyl)urea) (**1b**, 1.00 g, 3.0 mmol) was added to a refluxing THF solution (200 mL) of *o*-nitrophenylisocyanate (1.64 g, 10.0 mmol). The mixture was refluxed for 4 hours and the precipitate was filtered off and washed several times with methanol and diethyl ether and then dried over vacuum to give pure **1c** as a light yellow solid (1.65 g, 84 %). M.p.: 229 °C. ^{1}H NMR (400 MHz, DMSO-d_6, ppm): δ9.72 (s, 2H, Hd), 9.11 (s, 2H, Hc), 8.24 (d, J = 8.4 Hz, 2H, H7), 8.07 (d, J = 7.2 Hz, 2H, H10), 7.94 (s, 2H, Hb), 7.75 (d, J = 6.0 Hz, 2H, H3), 7.67 (m, 2H, H8), 7.38 (d, J = 8.0 Hz, 2H, H6), 7.19 (m, 2H, H9), 7.08 (m, 2H, H5), 6.98 (m, 2H, H4), 6.79 (s, 2H, Ha), 3.21 (m, 4H, CH2). ^{13}C NMR (100 MHz, DMSO-d_6), 155.8 (CO), 152.8 (CO), 137.7 (C), 134.9 (C), 133.7 (C), 128.4 (C), 125.4 (CH), 125.3 (CH, CH), 125.2 (CH), 122.6 (CH), 122.5 (CH), 122.2 (CH, CH), 39.5 (CH2). IR (KBr, ν/cm^{-1}): 3349, 3307, 3086, 1667, 1602, 1564, 1448, 1336, 1302. Anal. Calcd for $C_{30}H_{28}N_{10}O_8$: C, 54.88; H, 4.30; N, 21.33%. Found: C, 54.72; H, 4.44; N, 21.35%. ESI-MS: *m/z* 100%, 657.2 $[M + H]^+$; 60%, 679.2 $[M + Na]^+$.

1,1'-(Ethane-1,2-diyl)bis(3-(2-(3-(2-aminophenyl)ureido)phenyl)urea) (1d)

Hydrazine monohydrate (1.0 mL) was added dropwise to the suspension of 1,1'-(ethane-1,2-diyl)bis(3-(2-(3-(2-nitrophenyl)ureido)phenyl)urea) (**1c**, 1.00 g, 1.5 mmol) and Pd/C 10% (0.05 g, cat.) in methanol (150 mL). After refluxing for 12 hours, the solid was filtered off, dissolved in DMSO (30 mL), and filtered through Celite to remove Pd/C. The DMSO solution was poured in water (500 mL) and the precipitate thus obtained was filtered off, washed several times with ethanol and diethyl ether and then dried over vacuum to give **1d** as a brown solid (0.55g, 60 %). M.p.: 183 °C. ^{1}H NMR (400 MHz, DMSO-d_6, ppm): δ8.13 (s, 2H, Hd), 8.10 (s, 2H, Hc), 7.97 (s, 2H, Hb), 7.59 (d, J = 6.0 Hz, 2H, H7), 7.47 (d, J = 6.0 Hz, 2H, H10), 7.26 (d, J = 8.0 Hz, 2H, H3), 7.00 (m, 4H, H8 + H9), 6.84 (t, J = 6.8 Hz, 2H, H4),

6.72 (d, *J* = 6.4 Hz, 2H, H6), 6.64 (s, 2H, Ha), 6.55 (t, *J* = 6.4 Hz, 2H, H5), 4.79 (s, 4H, He), 3.21 (t, *J* = 2.4, 4H, CH2).^{13}C NMR (100 MHz, DMSO-d_6), 156.3 (CO), 153.8 (CO), 141.1 (C), 131.8 (C), 131.2 (C), 124.6 (C), 124.4 (CH), 124.1 (CH, CH), 123.6 (CH), 123.4 (CH), 116.6 (CH), 115.7 (CH, CH), 39.5 (CH2). IR (KBr, ν/cm^{-1}): 3347, 3299, 3115, 1617, 1569, 1505, 1476, 1262. Anal. Calcd for $C_{30}H_{32}N_{10}O_4$: C, 60.39; H, 5.41; N, 23.48%. Found: C, 60.72; H, 5.64; N, 23.45%. ESI-MS: *m/z* 100%, 597.3 $[M + H]^+$.

1,1'-(Ethane-1,2-diyl)bis(3-(2-(3-(2-(3-(4-nitrophenyl)ureido)phenyl)ureido)phenyl)urea) (L)

1,1'-(Ethane-1,2-diyl)bis(3-(2-(3-(2-aminophenyl)ureido)phenyl)urea) (**1d**, 0.5 g, 0.84 mmol) was added to a refluxing THF/DMSO (120 mL, v/v, 5:1) solution of *p*-nitrophenylisocyanate (0.33 g, 2.0 mmol). The mixture was refluxed for 4 hours and the precipitate was filtered off and washed several times with methanol and diethyl ether and then dried over vacuum to give pure **L** as a dark yellow solid (1.65 g, 84 %). M.p.: 233 °C. ^{1}H NMR (400 MHz, DMSO-d_6, ppm): δ 9.91 (s, 2H, Hf), 8.54 (s, 2H, He), 8.39 (s, 2H, Hd), 8.27 (s, 2H, Hc), 8.18 (d, *J* = 9.2 Hz, 4H, H12), 7.99 (s, 2H, Hb), 7.69 (d, *J* = 9.2 Hz, 4H, H11), 7.58 (m, 4H, H7 +H10), 7.47 (m, 4H, H3 + H6), 7.09 (m, 4H, H8 +H9), 7.00 (m, 4H, H4 +H5), 6.67 (s, 4H, Ha), 3.17 (t, J = 2.4, 4H, CH2). IR (KBr, ν/cm^{-1}): 3349, 3299, 3081, 1663, 1595, 1567, 1501, 1336, 1300. Anal. Calcd for $C_{44}H_{40}N_{14}O_{10}$: C, 57.14; H, 4.36; N, 21.20%. Found: C, 56.83; H, 4.24; N, 21.37%. ESI-MS: *m/z* 100%, 925.3 $[M + H]^+$; 60%, 947.3 $[M + Na]^+$.

S3. X-ray crystallography

Diffraction data were collected on a Bruker SMART APEX II diffractometer at 150 or 173 K with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). An empirical absorption correction using SADABS was applied for all data.[1] The structures were solved by direct methods using the SHELXS program.[2] All non-hydrogen atoms were refined anisotropically by full-matrix least-squares on F^2 by the use of the SHELXL program.[2] Hydrogen atoms bonded to carbon and nitrogen were included in idealized geometric positions with thermal parameters equivalent to 1.2 times those of the atom to which they were attached. Hydrogen atoms on the water oxygens were located from the difference Fourier map and then refined considering their chemical environments with restraints [O–H = 0.85(2) Å], with U(H) fixed at 0.08 Å^2. CCDC numbers 849100 – 849105.

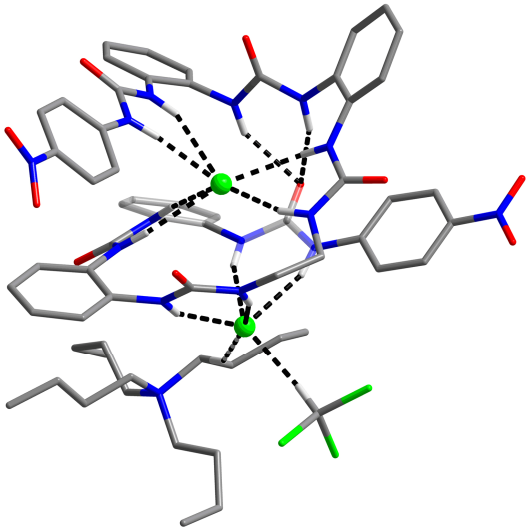


Fig. S1. The foldamer structure of complex **3**. Two Cl^- ions are surrounded by one ligand strand; a TBA^+ and a $CHCl_3$ molecule also bind with the anion. Only a *P* enantiomer is shown.

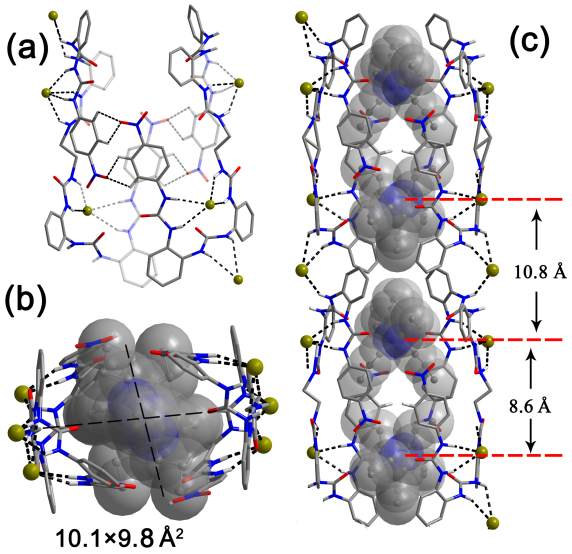


Fig. S2. (a) Illustration of the "face to face" dimerization of two ligands in **5** and the binding of six Br^- anions; (b, c) Two TPA^+ cations are encapsulated in the molecular barrel; (d) Infinite tube connected by Br^- ions.

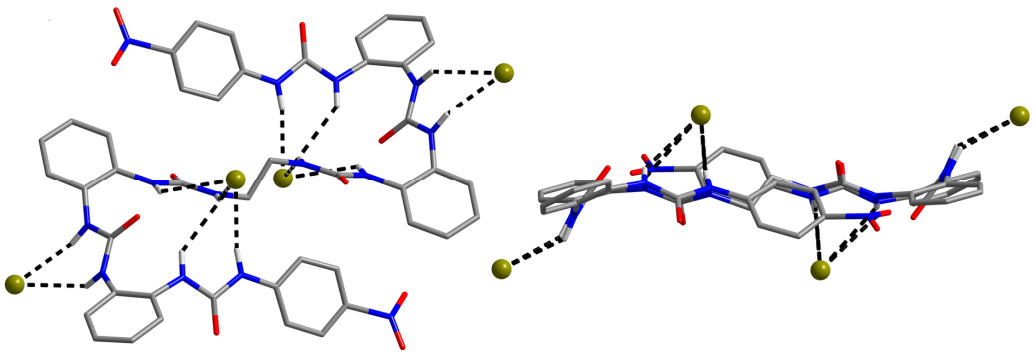


Fig. S3. The flat structure of complex **6** [$(TBA)_4LBr_4$] and its side view.

Table S1. Crystal data and structural refinement of **1-6**.

	1	**2**	**3**
Formula	$C_{76}H_{122}Cl_4N_{18}O_{11}$	$C_{80}H_{124}Cl_3N_{17}O_{10}$	$C_{82}H_{124}Cl_8N_{16}O_{11}$
M	1605.72	1590.31	1793.57
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	*P*-1	*C2/c*	*P-1*
a /Å	16.207 (4)	32.425 (8)	12.995 (2)
b /Å	18.232 (4)	19.215 (5)	18.961 (3)
c /Å	19.617 (5)	28.184 (7)	21.692 (4)
α /°	99.111 (4)	90.00	101.726 (3)
β /°	103.442 (5)	98.692 (4)	106.372 (3)
γ /°	105.631 (4)	90.00	102.616 (3)
V /Å^3	5376 (2)	17358 (8)	4800.1 (14)
Z	2	8	2
T /K	150 (2)	100 (2)	150 (2)
F(000)	1720	6832	1904
D_{calc} /g cm^{-3}	1.011	1.217	1.241
μ /mm^{-1}	0.17	0.17	0.30
R_{int}	0.047	0.099	0.072
Data/restraints/param	18716/1/1018	15068/33/1027	16924/0/1064
GOF	0.999	1.794	1.221
R_1 [$I > 2\sigma(I)$]	0.078	0.146	0.103
wR_2 [$I > 2\sigma(I)$]	0.227	0.388	0.304

	4	**5**	**6**
Formula	$C_{76}H_{120}Br_4N_{18}O_{10}$	$C_{80}H_{124}Br_3N_{17}O_{10}$	$C_{108}H_{124}Br_4N_{18}O_{11}$
M	1765.54	1723.69	2232.39
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	*C2/c*	*P2(1)/n)*
a /Å	11.952 (3)	32.939(3)	12.2557(18)
b /Å	28.436 (8)	19.383 (2)	37.945(6)
c /Å	12.614 (4)	28.226 (3)	13.0316(19)
α /°	90.00	90.00	90.00
β /°	90.341 (4)	97.879 (2)	96.945(2)
γ /°	90.00	90.00	90.00
V /Å^3	4283 (2)	17851 (3)	6015.8(15)
Z	2	8	2
T /K	100 (2)	100 (2)	100 (2)
F(000)	1844	7264	2376
D_{calc} /g cm^{-3}	1.369	1.283	1.399
μ /mm^{-1}	1.94	1.42	1.40
R_{int}	0.065	0.053	0.064
Data/restraints/param	7455/0/495	15689/6/1073	10560/18/659
GOF	1.04	1.04	1.688
R_1 [$I > 2\sigma(I)$]	0.043	0.080	0.109
wR_2 [$I > 2\sigma(I)$]	0.113	0.263	0.295

Table S2. Selected hydrogen bonds in compound **1**.

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (°)
N13–H13···Cl4	0.86	2.29	3.153(3)	166.7
N12–H12···Cl4	0.86	2.47	3.300(4)	158.0
N9–H9···Cl4	0.86	2.67	3.475(4)	153.2
N8–H8···Cl4	0.86	2.32	3.179(4)	167.0
N11–H11···Cl3	0.86	2.48	3.175(3)	136.0
N10–H10···Cl3	0.86	2.65	3.315(3)	133.2
N5–H5···Cl2	0.86	2.53	3.241(4)	137.9
N4–H4···Cl1	0.86	3.43	3.583(4)	93.1
N7–H7···Cl1	0.86	2.30	3.159(4)	164.4
N6–H6···Cl1	0.86	2.57	3.386(4)	154.0
N3–H3···Cl1	0.86	2.53	3.336(3)	152.7
N2–H2···Cl1	0.86	2.36	3.147(4)	148.3
O11–H11C···Cl3	0.86	2.49	3.320(4)	167.7
O11–H11B···Cl2	0.86	2.51	3.276(4)	150.5

Table S3. Hydrogen bonds around the Cl^- ions in compound **2**.

D−H···A	*d*(D−H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (°)
N13–H13···Cl3	0.86	2.26	3.110(9)	162.8
N12–H12···Cl3	0.86	2.55	3.364(8)	153.8
N9–H9···Cl3	0.86	2.61	3.430(7)	155.7
N8–H8···Cl3	0.86	2.43	3.220(8)	149.3
N7–H7···Cl1	0.86	2.42	3.212(7)	150.3
N6–H6···Cl1	0.86	2.61	3.427(7)	154.3
N3–H3···Cl1	0.86	2.53	3.344(8)	154.8
N2–H2···Cl1	0.86	2.28	3.120(8)	160.2
N11–H11···Cl2	0.86	2.59	3.247(8)	132.1
N10–H10···Cl2	0.86	2.83	3.363(7)	120.2
N5–H5···Cl2	0.86	2.83	3.408(7)	125.0
N4–H4···Cl2	0.86	2.57	3.231(7)	132.3

Table S4. Selected hydrogen bonds in compound **3**.

D−H···A	*d*(D−H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (°)
N2–H2···Cl1	0.86	2.39	3.222(5)	158.8
N3–H3···Cl1	0.86	2.56	3.388(5)	156.1
N6–H6···Cl1	0.86	2.54	3.370(5)	156.7
N7–H7···Cl1	0.86	2.49	3.327(6)	158.8
N4–H4···Cl2	0.86	2.29	3.153(5)	167.0
N5–H5···Cl2	0.86	2.48	3.310(5)	158.2
N8–H8···Cl2	0.86	2.39	3.210(6)	154.4
N9–H9···Cl2	0.86	2.41	3.212(5)	152.2
N12–H12···Cl2	0.86	2.60	3.417(6)	153.9
N13–H13···Cl2	0.86	2.29	3.158(6)	168.6
N10–H10···O3	0.86	2.20	2.995(7)	150.6
N11–H11···O3	0.86	2.12	2.927(7)	151.8
C77–H77···Cl1	1.00	2.48	3.475(9)	175.5
C61–H61B···Cl1	0.99	2.77	3.624(7)	144.9

Table S5. Hydrogen bonds around the Br^- ions in compound **4**.

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (°)
N5–H5···Br2	0.86	2.62	3.447(3)	156.1
N4–H4···Br2	0.86	2.51	3.369(3)	165.7
N7–H7···Br1	0.86	2.55	3.372(3)	156.2
N6–H6···Br1	0.86	2.56	3.398(3)	158.8
N3–H3···Br1	0.86	2.62	3.449(3)	157.4
N2–H2···Br1	0.86	2.65	3.485(3)	158.3

Table S6. Selected hydrogen bonds in compound **5**.

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (°)
N1–H11A···Br3	0.86	2.76	3.390(6)	129.6
N10–H10A···Br3	0.86	2.99	3.497(6)	118.6
N4–H4···Br3	0.86	2.73	3.378(6)	131.5
N5–H5A···Br3	0.86	2.97	3.530(6)	123.6
N13–H13···Br2	0.86	2.42	3.273(7)	162.5
N12–H12A···Br2	0.86	2.71	3.526(6)	155.3
N9–H9A···Br2	0.86	2.76	3.575(6)	155.3
N8–H8···Br2	0.86	2.63	3.361(7)	140.9
N6–H6A···Br1	0.86	2.78	3.591(6)	154.5
N3–H3A···Br1	0.86	2.65	3.473(6)	156.8
N2–H2A···Br1	0.86	2.42	3.258(6)	160.2
N7–H7A···Br1	0.86	2.57	3.347(6)	147.5

Table S7. Hydrogen bonds around the Br^- ions in compound **6**.

D–H···A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(DHA) (°)
N5–H5···Br2	0.86	2.52	3.272(6)	144.4
N4–H4···Br2	0.86	2.63	3.342(6)	138.8
N2–H2···Br1	0.86	2.49	3.346(7)	164.4
N3–H3···Br1	0.86	3.2	3.924(6)	141.3
N6–H6···Br1	0.86	3.26	3.912(6)	133
N7–H7···Br1	0.86	2.55	3.350(6)	152

S4. ^{1}H NMR studies

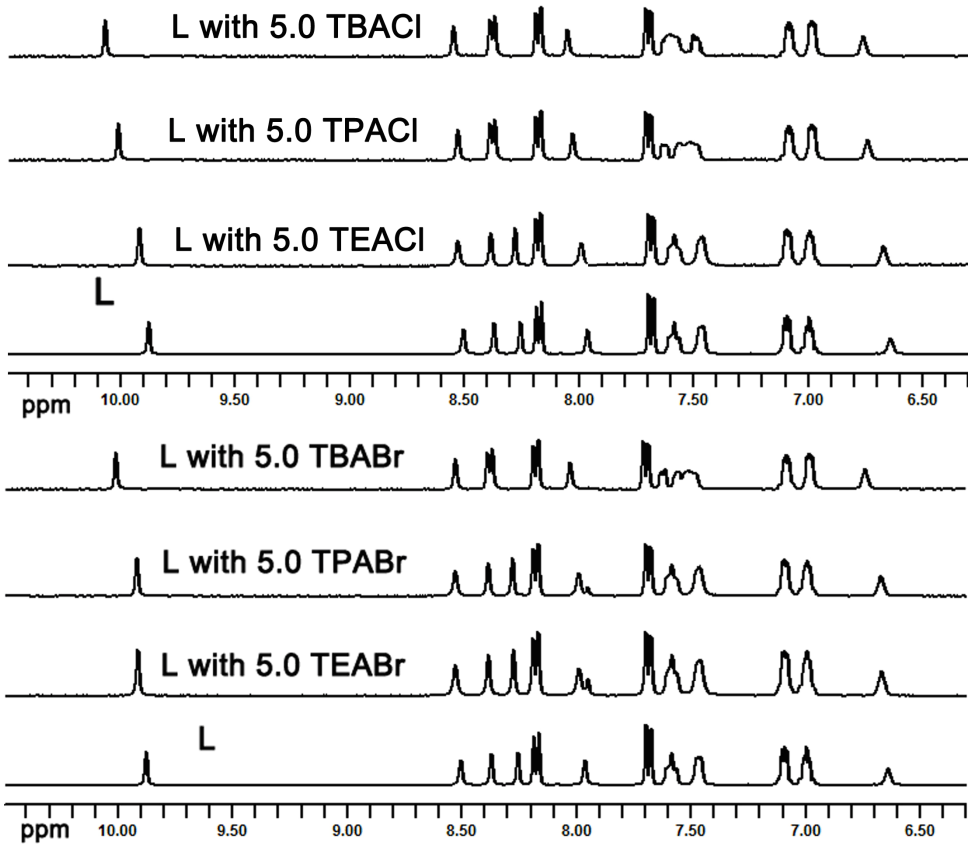


Fig. S4. Countercation effects on the halide binding in DMSO-d_6.

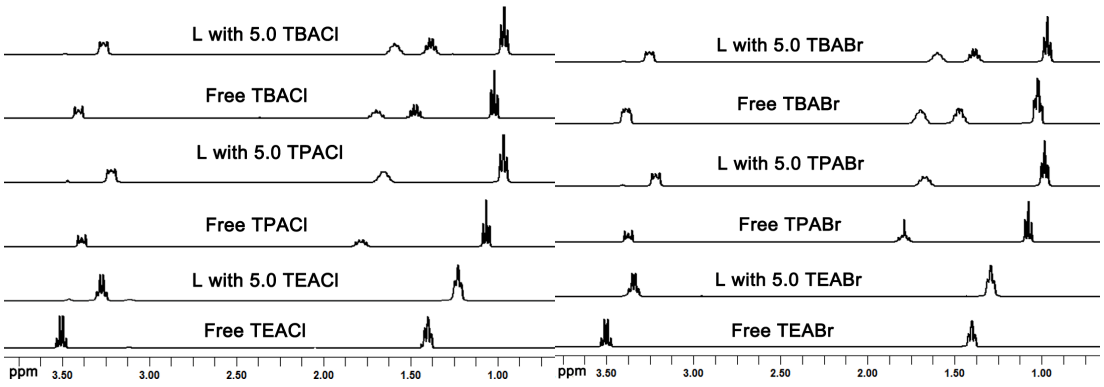


Fig. S5. ^{1}H NMR spectra of the tetraalkylammonium halides in the presence of ligand L in $CDCl_3$.

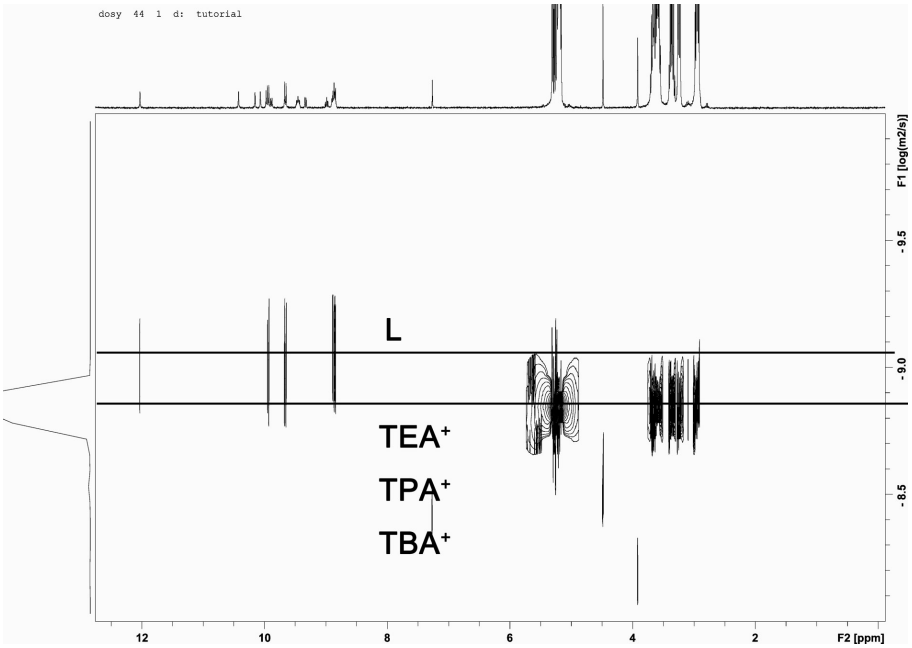


Fig. S6. ^{1}H DOSY NMR spectra of **L** with 6.0 times $(R_4N^+)Cl^-$ in CD_2Cl_2 at 298 K. There are two horizontal lines corresponding to [L-anions]$^{n-}$ and [cation]$^+$, respectively.

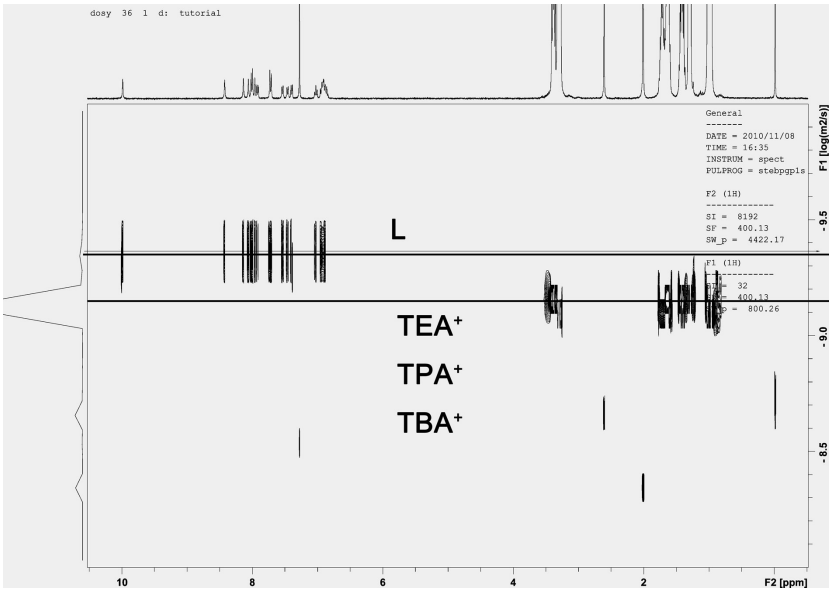


Fig. S7. ^{1}H DOSY NMR spectra of **L** with 6.0 times $(R_4N^+)Cl^-$ in $CDCl_3$ at 298 K.

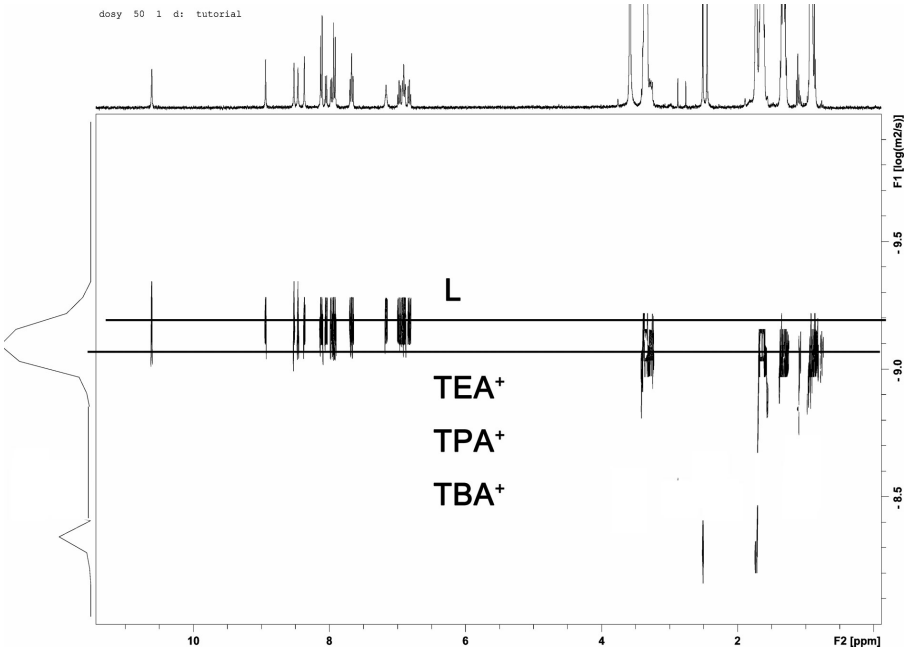


Fig. S8. ^{1}H DOSY NMR spectra of **L** with 6.0 times of $(R_4N^+)Cl^-$ in THF-d_8 at 298 K.

S5. Computations

Cartesian coordinates for the optimized geometry of **L**:

O	-0.12976	0.71226	7.68698	C	0.00595	2.63634	6.36377
O	0.72089	2.56737	8.58954	C	0.44551	3.95905	6.24329
O	0.7394	6.52315	2.91675	H	0.92415	4.43763	7.08745
O	0.22602	6.80336	-3.81823	C	0.26711	4.64317	5.0456
O	0.7658	0.56639	-2.76085	H	0.6229	5.65555	4.93164
N	0.2107	1.93419	7.61971	C	-0.36396	3.99657	3.96116
N	-0.61283	4.63171	2.73093	C	-0.79296	2.6585	4.09889
H	-1.16383	4.09391	2.07634	H	-1.24994	2.13149	3.26687
N	-0.67535	6.2744	1.08741	C	-0.61241	1.97657	5.29517
H	-1.55413	5.85204	0.80922	H	-0.93872	0.9502	5.39338
N	-0.03006	6.21382	-1.574	C	-0.11591	5.86589	2.29732
H	0.01249	5.44068	-0.92333	C	-0.32956	7.5114	0.43631
N	-0.07339	4.57848	-3.198	C	-0.31314	8.72175	1.13528
H	-0.33392	3.95883	-2.44233	H	-0.51801	8.71808	2.1981
N	-0.99518	2.00244	-3.29993	C	-0.01539	9.9121	0.46845
H	-1.98682	2.15849	-3.1613	H	0.00202	10.84821	1.01531
N	-1.09223	0.657	-1.39883	C	0.24975	9.8858	-0.90498
H	-2.00963	1.03937	-1.22623	H	0.47208	10.80752	-1.43251

C	0.24548	8.68407	-1.61689	C	-0.00595	-2.63634	-6.36377
H	0.45766	8.65765	-2.67509	C	-0.44551	-3.95905	-6.24329
C	-0.03193	7.47953	-0.94787	H	-0.92415	-4.43763	-7.08745
C	0.06037	5.93425	-2.93613	C	-0.26711	-4.64317	-5.0456
C	0.02996	3.91857	-4.44084	H	-0.6229	-5.65555	-4.93164
C	0.5474	4.51263	-5.60387	C	0.36396	-3.99657	-3.96116
H	0.85833	5.5464	-5.57494	C	0.79296	-2.6585	-4.09889
C	0.63677	3.76295	-6.78016	H	1.24994	-2.13149	-3.26687
H	1.04179	4.23237	-7.67079	C	0.61241	-1.97657	-5.29517
C	0.21611	2.42915	-6.8246	H	0.93872	-0.9502	-5.39338
H	0.29063	1.84464	-7.73337	C	0.11591	-5.86589	-2.29732
C	-0.31591	1.84334	-5.67293	C	0.32956	-7.5114	-0.43631
H	-0.66029	0.81716	-5.69598	C	0.31314	-8.72175	-1.13528
C	-0.41021	2.57378	-4.48762	H	0.51801	-8.71808	-2.1981
C	-0.37089	1.03591	-2.51471	C	0.01539	-9.9121	-0.46845
C	-0.55228	-0.30894	-0.44305	H	-0.00202	-10.84821	-1.01531
H	-0.14206	-1.16535	-0.98847	C	-0.24975	-9.8858	0.90498
H	-1.36847	-0.65711	0.19403	H	-0.47208	-10.80752	1.43251
O	0.12976	-0.71226	-7.68698	C	-0.24548	-8.68407	1.61689
O	-0.72089	-2.56737	-8.58954	H	-0.45766	-8.65765	2.67509
O	-0.7394	-6.52315	-2.91675	C	0.03193	-7.47953	0.94787
O	-0.22602	-6.80336	3.81823	C	-0.06037	-5.93425	2.93613
O	-0.7658	-0.56639	2.76085	C	-0.02996	-3.91857	4.44084
N	-0.2107	-1.93419	-7.61971	C	-0.5474	-4.51263	5.60387
N	0.61283	-4.63171	-2.73093	H	-0.85833	-5.5464	5.57494
H	1.16383	-4.09391	-2.07634	C	-0.63677	-3.76295	6.78016
N	0.67535	-6.2744	-1.08741	H	-1.04179	-4.23237	7.67079
H	1.55413	-5.85204	-0.80922	C	-0.21611	-2.42915	6.8246
N	0.03006	-6.21382	1.574	H	-0.29063	-1.84464	7.73337
H	-0.01249	-5.44068	0.92333	C	0.31591	-1.84334	5.67293
N	0.07339	-4.57848	3.198	H	0.66029	-0.81716	5.69598
H	0.33392	-3.95883	2.44233	C	0.41021	-2.57378	4.48762
N	0.99518	-2.00244	3.29993	C	0.37089	-1.03591	2.51471
H	1.98682	-2.15849	3.1613	C	0.55228	0.30894	0.44305
N	1.09223	-0.657	1.39883	H	0.14206	1.16535	0.98847
H	2.00963	-1.03937	1.22623	H	1.36847	0.65711	-0.19403

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