Electronic Supplementary Information

Cation-Chloride Cotransport Mediated by An Ion Pair Transporter

Jun Zhu,[1,2] Xu-Dong Wang,[1,*] Jian Luo,[1] Yu-Fei Ao,[1,2] Qi-Qiang Wang,[1,2] De-Xian Wang[1,2,*]

[1] Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100190, China

[2] School of Chemical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China

wangxd@iccas.ac.cn; dxwang@iccas.ac.cn

Contents

1. General methods

Reagents for synthesis and analysis were purchased from J&K or Sigma-Aldrich. A Mini-Extruder used for vesicle preparation, egg yolk phosphatidylcholine (EYPC). ^{1}H and ^{13}C NMR spectra were recorded on Bruker 400 or 500 MHz NMR spectrometer. Chemical shifts are reported in ppm and referenced to tetramethylsilane (TMS) or the residual solvent resonance. X-ray crystallography were performed at the Analytical Laboratory of the Institute. All solvents were dried according to standard procedures prior to use. All other major chemicals were obtained from commercial sources and used without further purification.

2. ^{1}H NMR titration and data analysis

2.1 ^{1}H NMR titration and data analysis for binding of 1 with cations

The stock solution of **1** (1.05×10^{-2} M) in deuterated acetonitrile was prepared, then an initial spectrum was recorded and additional spectra were obtained after aliquots of salt ($LiClO_4$, $NaClO_4$, KPF_6, $Mg(ClO_4)_2$, $Ca(ClO_4)_2 \cdot 4H_2O$) solution (salt solutions were prepared by using host stock solution as solvent to avoid dilution). As the proton ***a***, ***b***, ***e*** are the most sensitive protons towards cation binding, these three protons were applied to the data fitting program to obtain the cation binding constants. The binding constants were calculated by *Bindfit v0.5* program[1] using a 1:1 binding stoichiometry for [**1**+M^{2+}] complex.

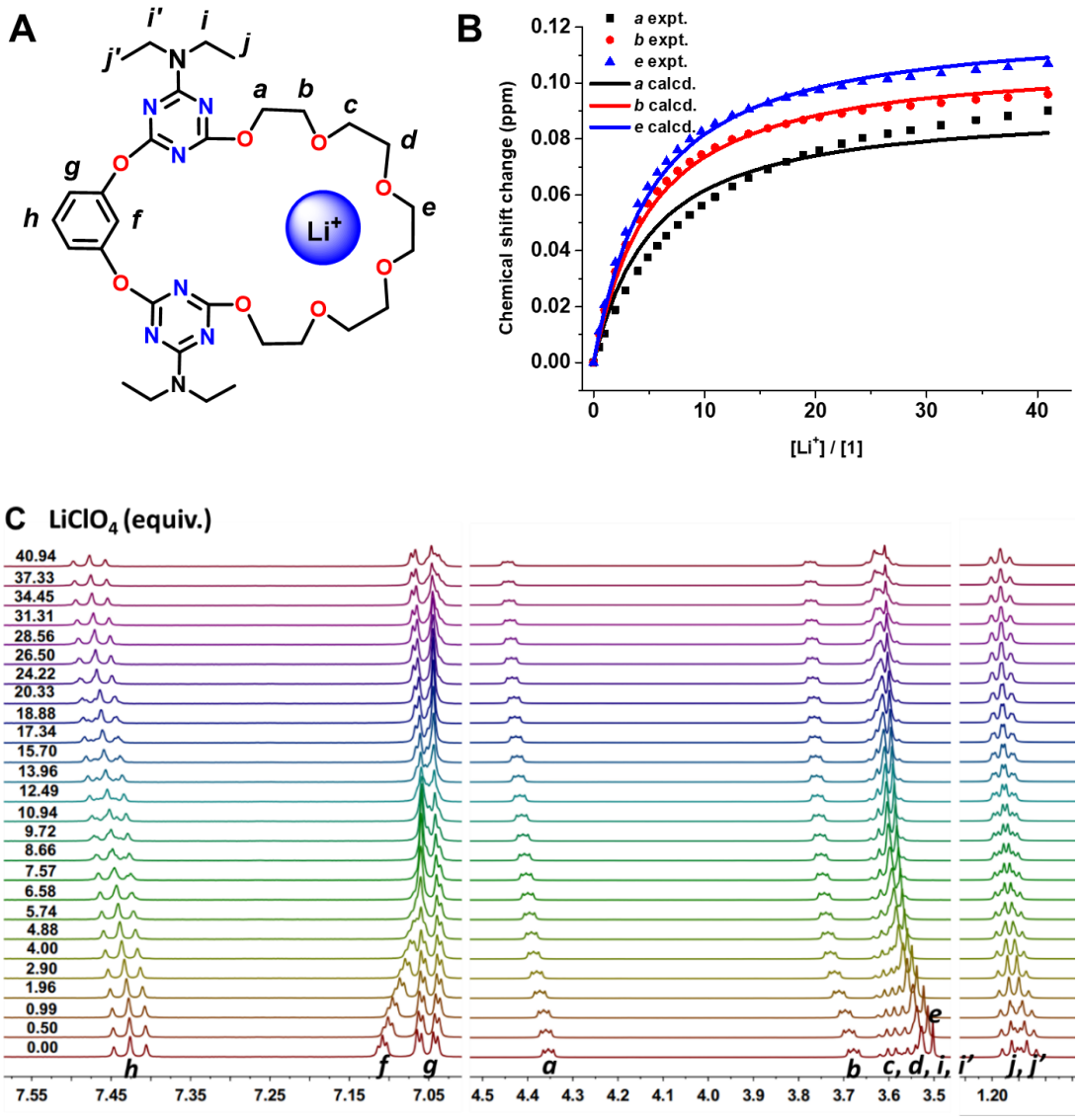


Figure S1. (a) A schematic binding mode of [**1**·Li^+] complex, (b)The fitting of the NMR titration data by *Bindfit v0.5* program, (c) ^{1}H NMR titration of **1** (1.05×10^{-2} M) with increasing equivalents of $LiClO_4$ in CD_3CN.

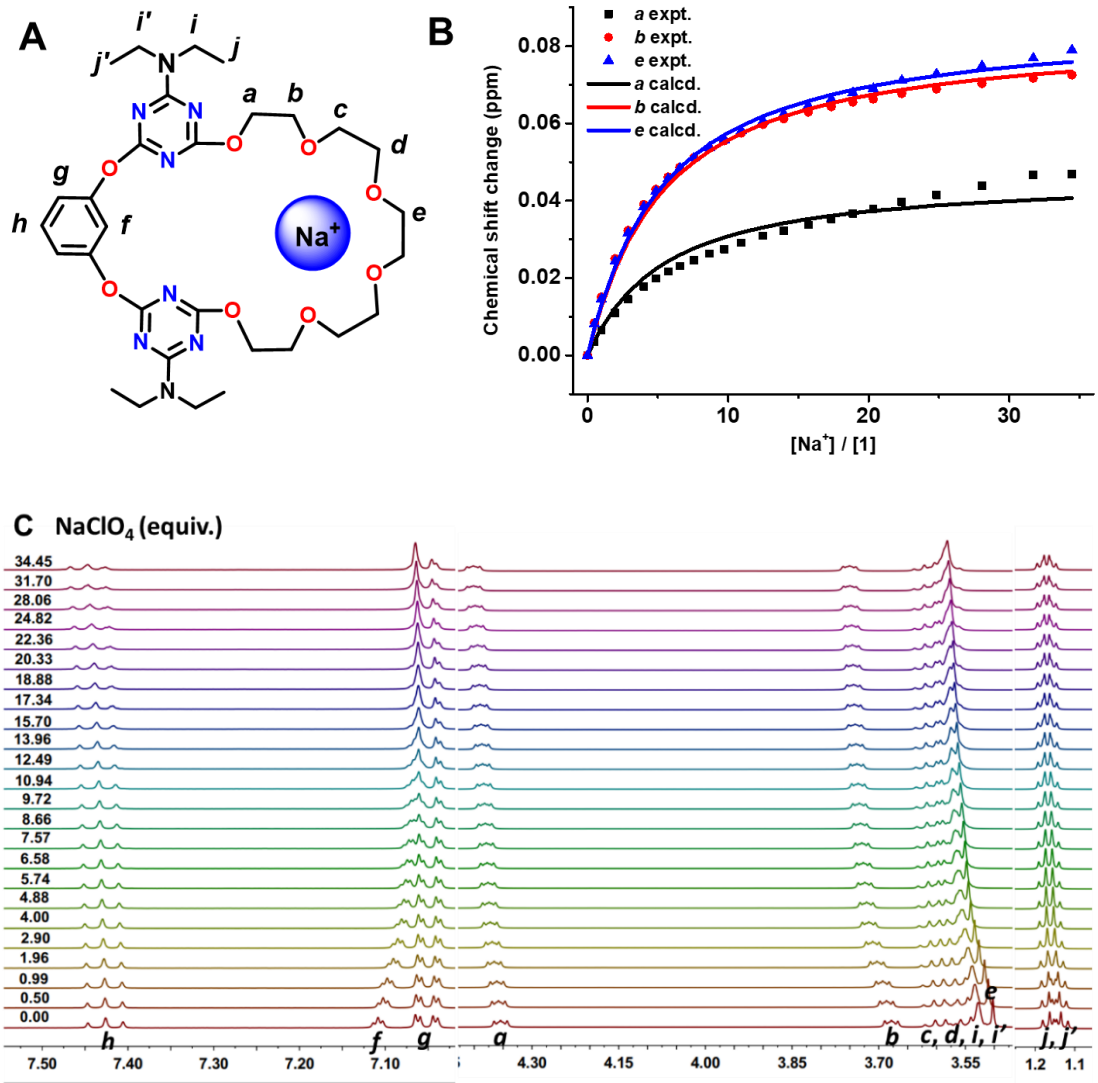


Figure S2. (a) A schematic binding mode of [**1**·Na^+] complex, (b)The fitting of the NMR titration data by *Bindfit v0.5* program, (c) ^{1}H NMR titration of **1** (1.05×10^{-2} M) with increasing equivalents of $NaClO_4$ in CD_3CN.

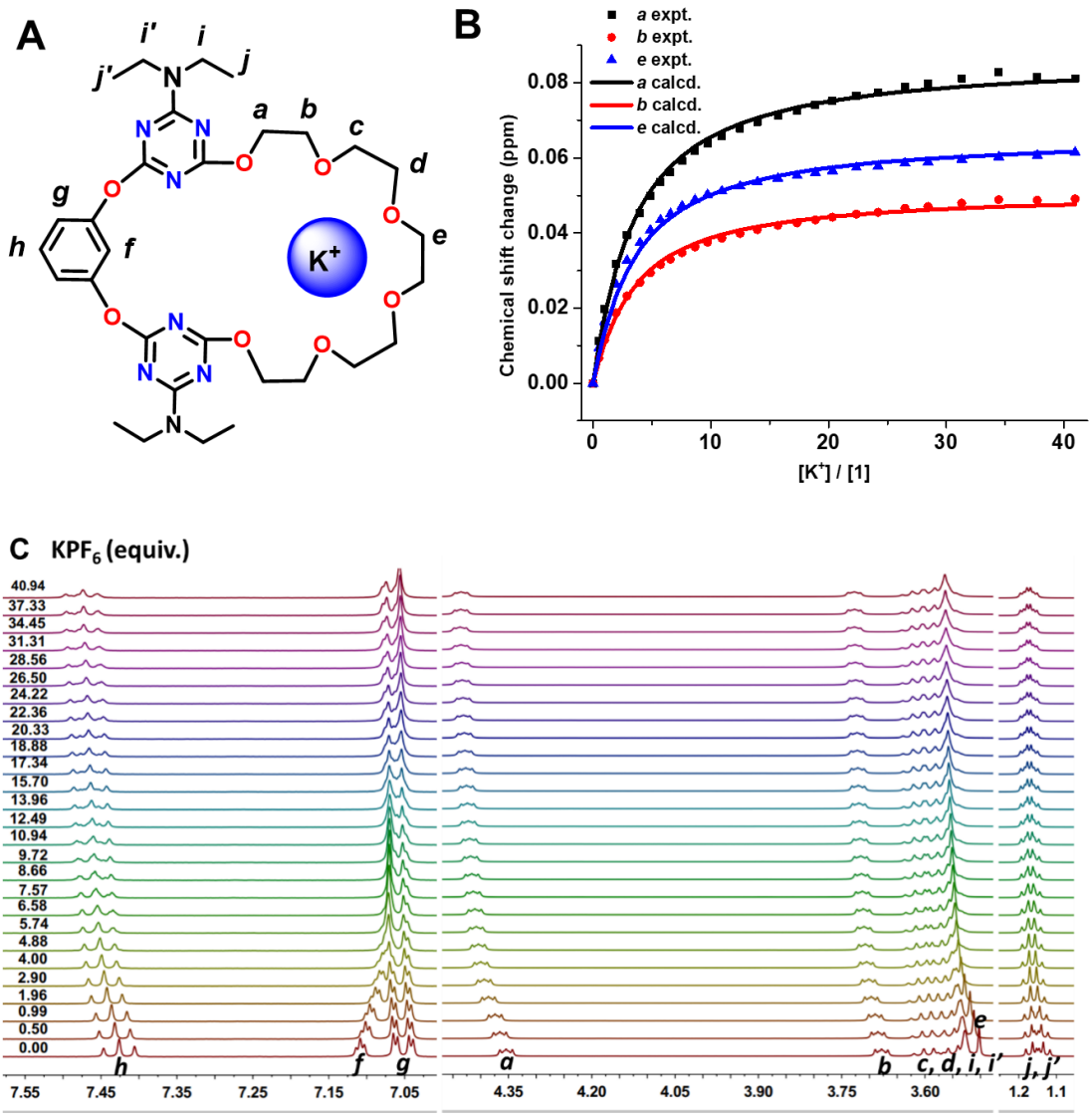


Figure S3. (a) A schematic binding mode of [**1**·K^+] complex, (b)The fitting of the NMR titration data by *Bindfit v0.5* program, (c) ^{1}H NMR titration of **1** (1.05×10^{-2} M) with increasing equivalents of KPF_6 in CD_3CN.

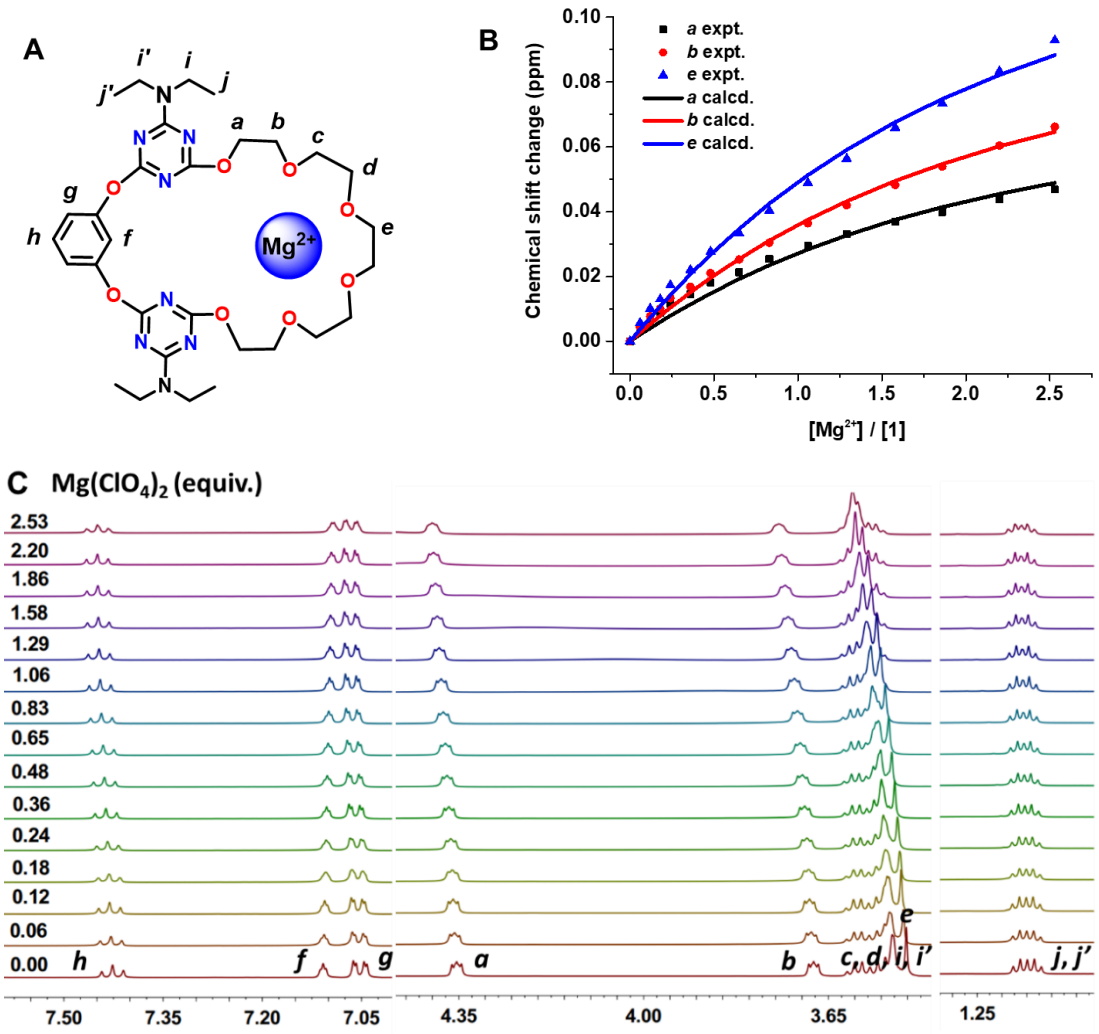


Figure S4. (a) A schematic binding mode of [**1**·Mg^{2+}] complex, (b)The fitting of the NMR titration data by *Bindfit v0.5* program, (c) ^{1}H NMR titration of **1** (1.05×10^{-2} M) with increasing equivalents of $Mg(ClO_4)_2$ in CD_3CN.

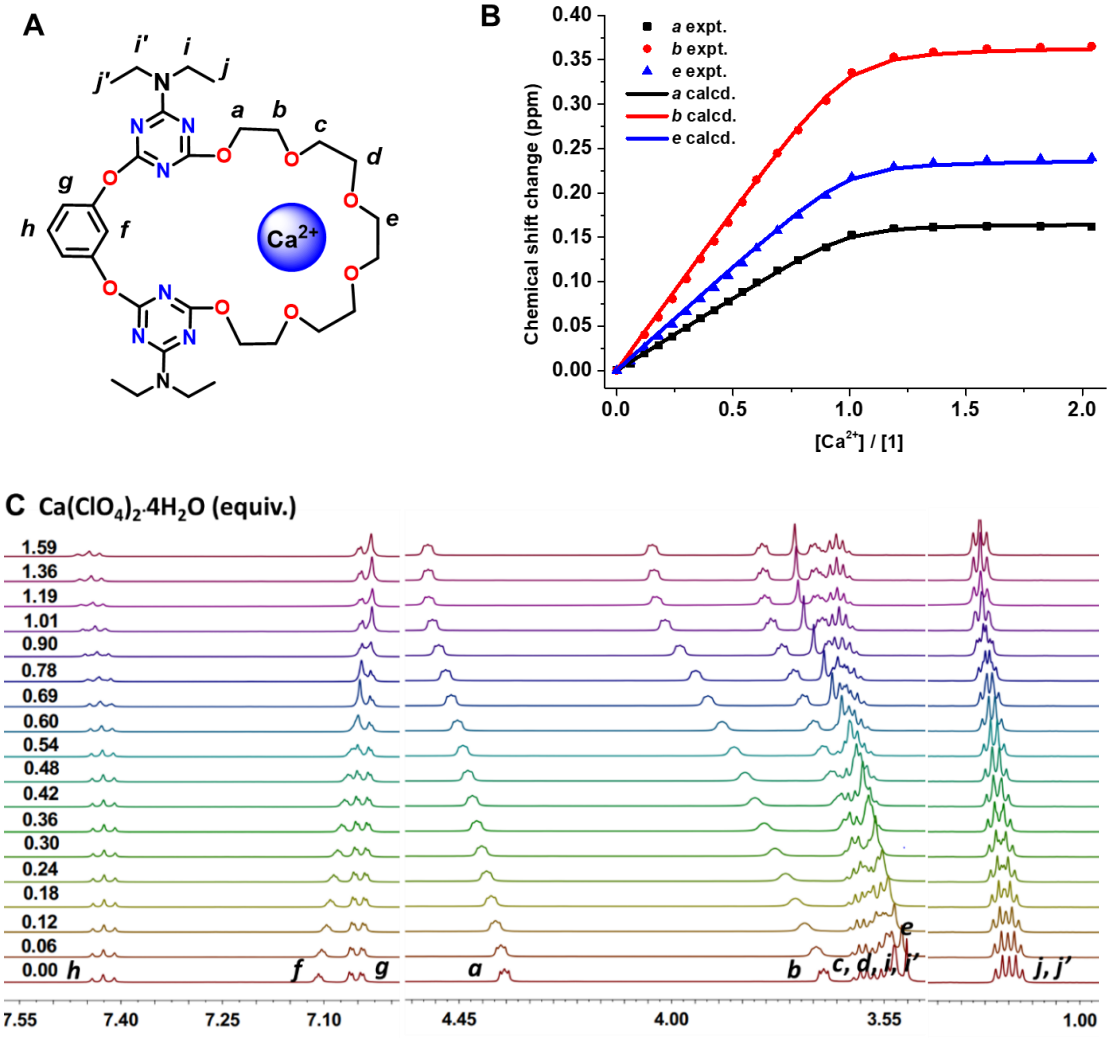


Figure S5. (a) A schematic binding mode of [**1**·Ca^{2+}] complex, (b)The fitting of the NMR titration data by *Bindfit v0.5* program, (c) ^{1}H NMR titration of **1** (1.05×10^{-2} M) with increasing equivalents of $Ca(ClO_4)_2$ in CD_3CN.

Table S1. Association constants for **1** binding alkaline earth metal cation.[a]

Transporter		Li^+	Na^+	K^+	Mg^{2+}	Ca^{2+}
1	K (M^{-1})	21	20	32	65	9383

[a] association constants were determined by ^{1}H NMR titration in CD_3CN, and fitted according to 1:1 binding model of *Bindfit v0.5* program.

2.2 ^{1}H NMR titration and data analysis for binding of 1 with anions

The stock solution of **1** (1.05×10^{-2} M) in deuterated acetonitrile was prepared, then an initial spectrum was recorded and additional spectra were obtained after aliquots of salt (TBACl, TBABr, TBAI, $TBAClO_4$) solution (salt solutions were prepared by using host stock solution as solvent to avoid dilution).

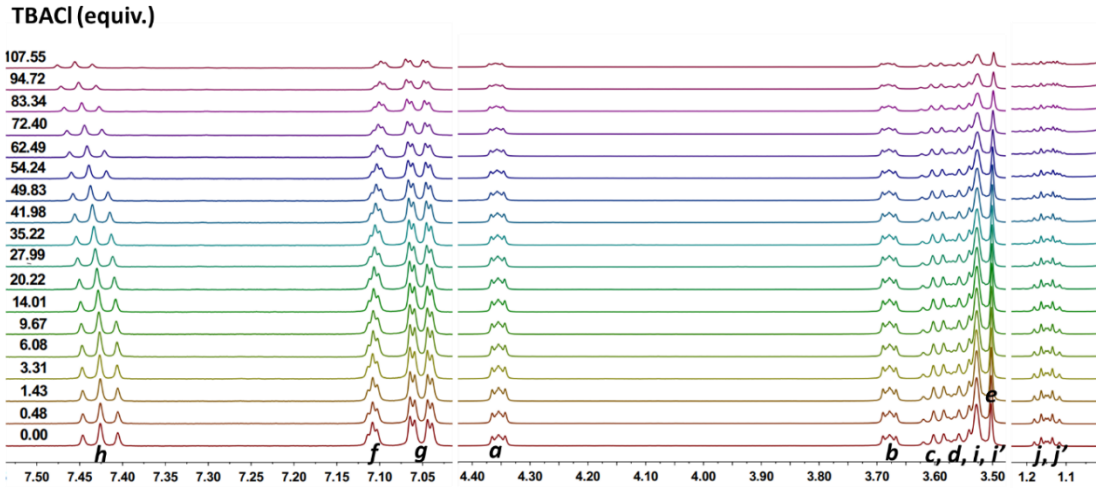


Figure S6. ^{1}H NMR titration of **1** (1.05×10^{-2} M) with increasing equivalents of TBACl in CD_3CN.

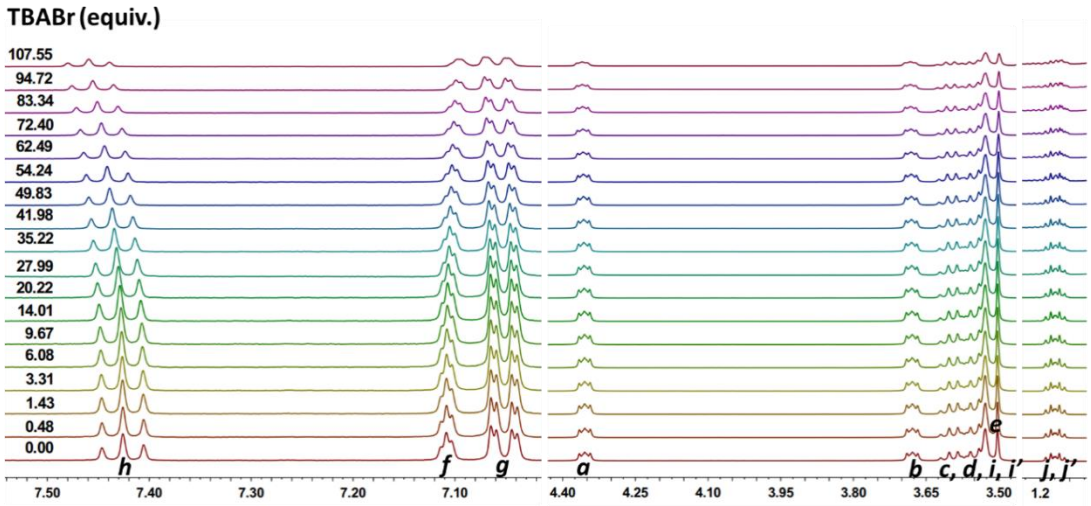


Figure S7. ^{1}H NMR titration of **1** (1.05×10^{-2} M) with increasing equivalents of TBABr in CD_3CN.

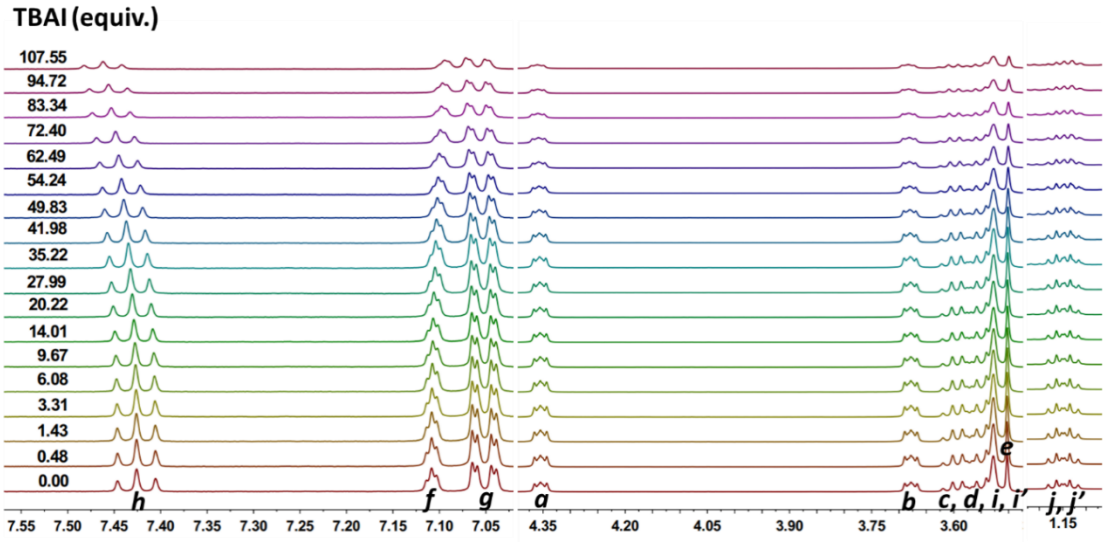


Figure S8. ^{1}H NMR titration of **1** (1.05×10^{-2} M) with increasing equivalents of TBAI in CD_3CN.

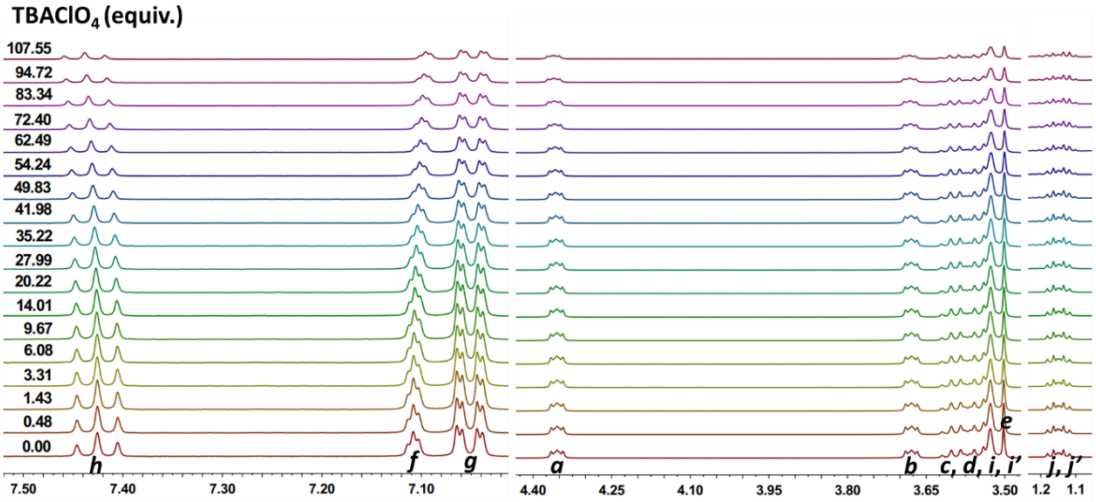


Figure S9. ^{1}H NMR titration of **1** (1.05×10^{-2} M) with increasing equivalents of $TBAClO_4$ in CD_3CN.

2.3 ^{1}H NMR titration and data analysis for binding of 1 with ion-pair

Based on calculation, when 2.0 eq. M^+/M^{2+} was added into the stock solution of **1**. The titration method is similar to above. An initial spectrum was recorded and additional spectra were obtained after aliquots of salt (TBAX, X = Cl^-, Br^-, I^-).

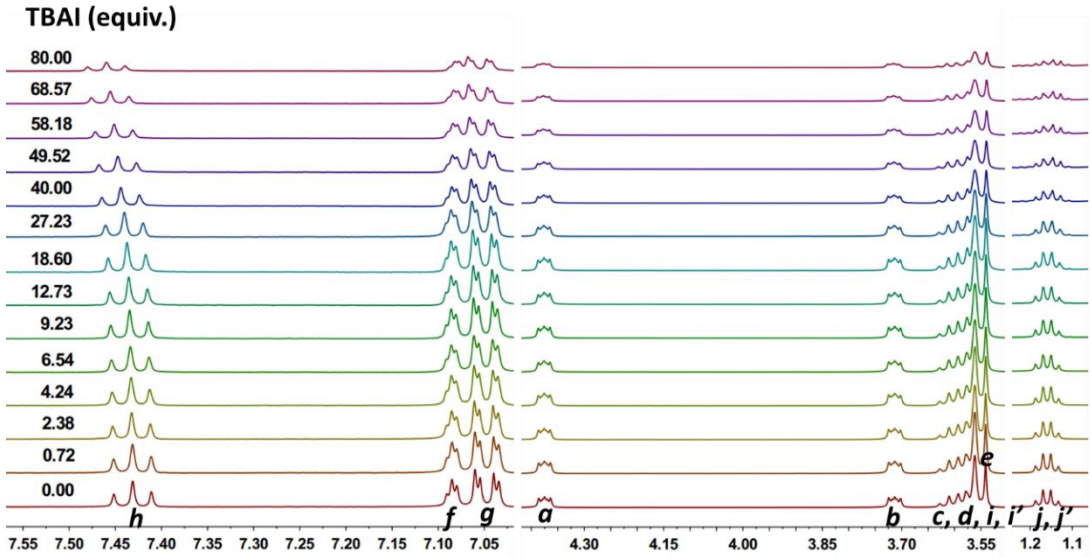


Figure S10. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $LiClO_4$ (2.10×10^{-2} M) with increasing equivalents of TBAI in CD_3CN.

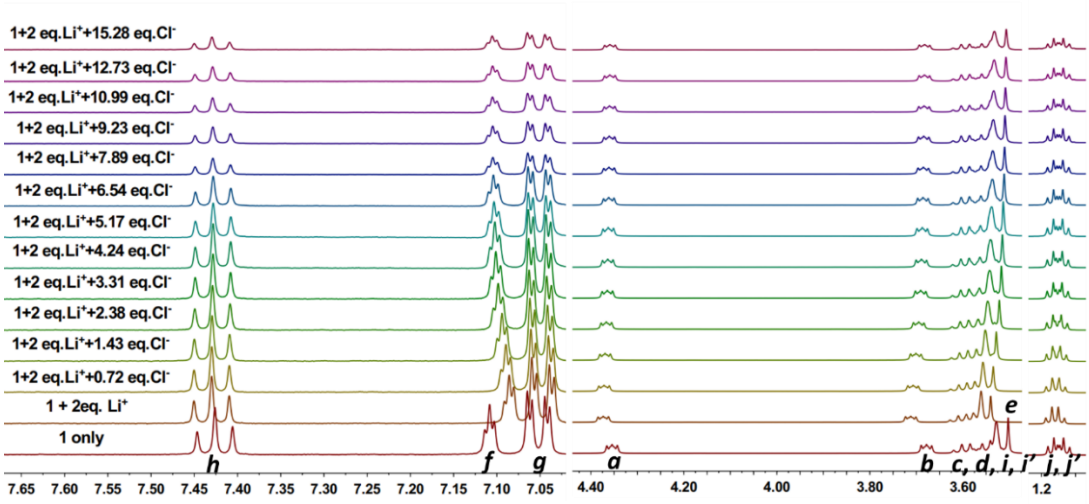


Figure S11. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $LiClO_4$ (2.10×10^{-2} M) with increasing equivalents of TBACl in CD_3CN.

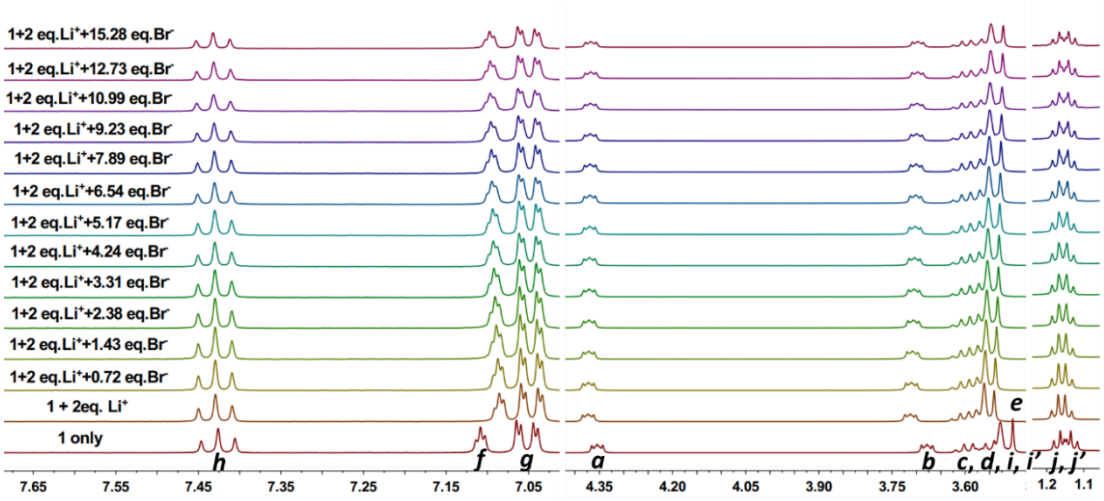


Figure S12. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $LiClO_4$ (2.10×10^{-2} M) with increasing equivalents of TBABr in CD_3CN.

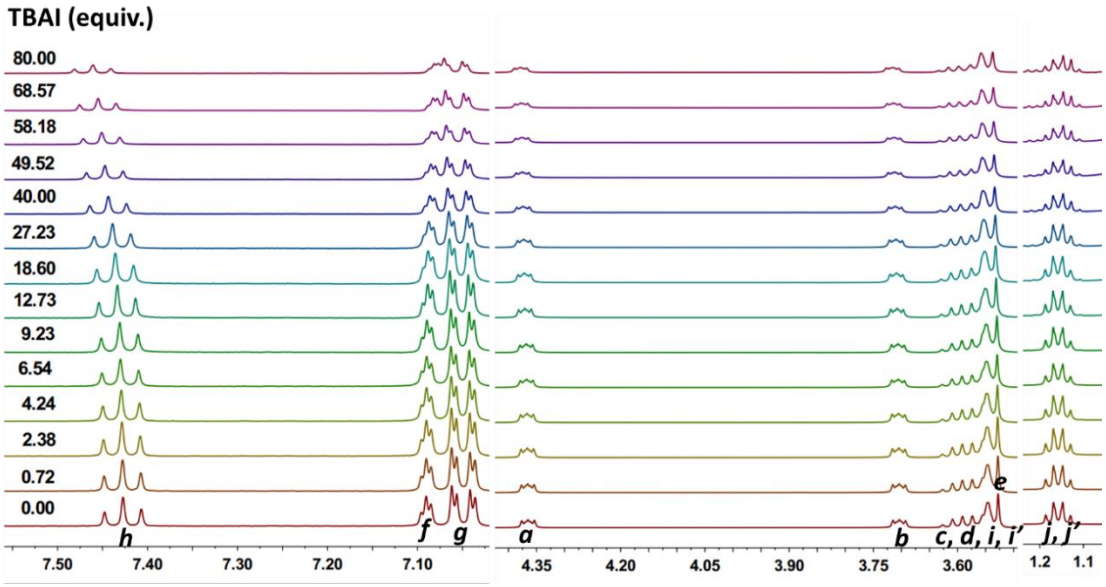


Figure S13. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $NaClO_4$ (2.10×10^{-2} M) with increasing equivalents of TBAI in CD_3CN.

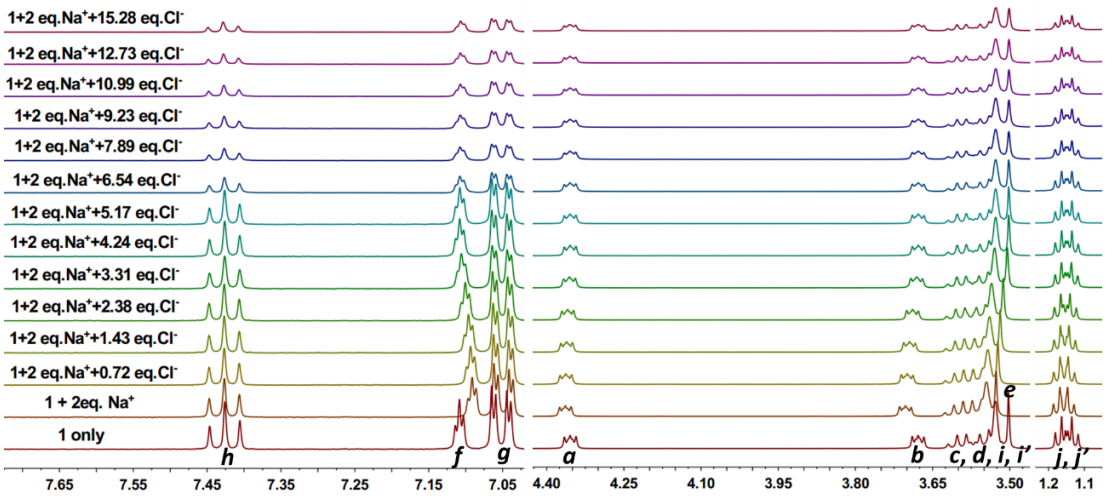


Figure S14. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $NaClO_4$ (2.10×10^{-2} M) with increasing equivalents of TBACl in CD_3CN.

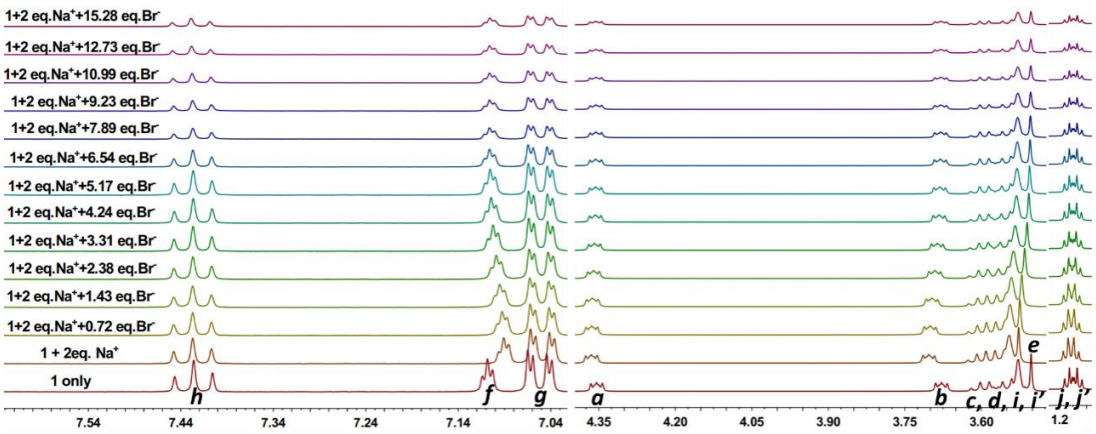


Figure S15. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $NaClO_4$ (2.10×10^{-2} M) with increasing equivalents of TBABr in CD_3CN.

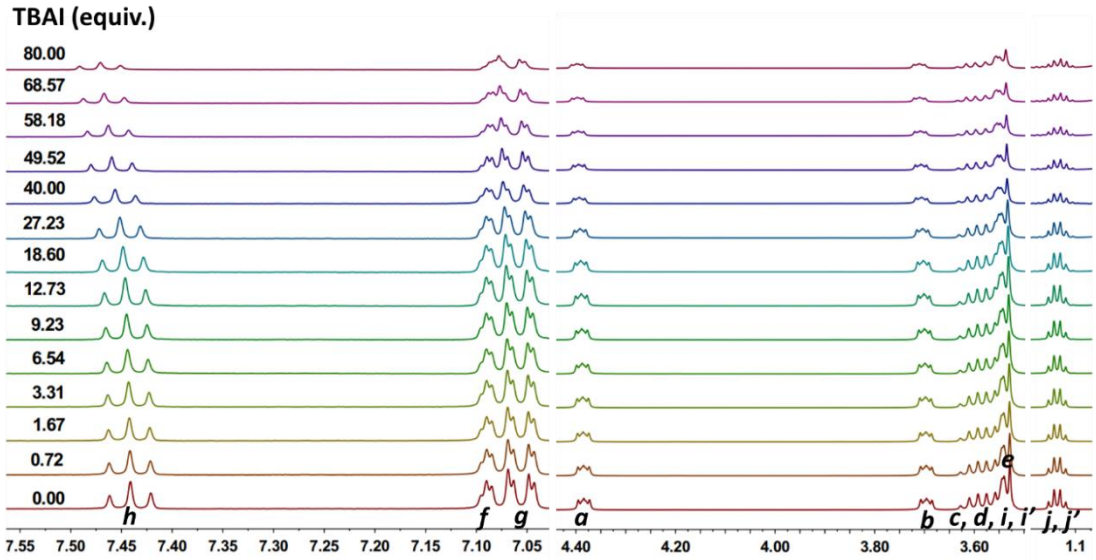


Figure S16. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and KPF_6 (2.10×10^{-2} M) with increasing equivalents of TBAI in CD_3CN.

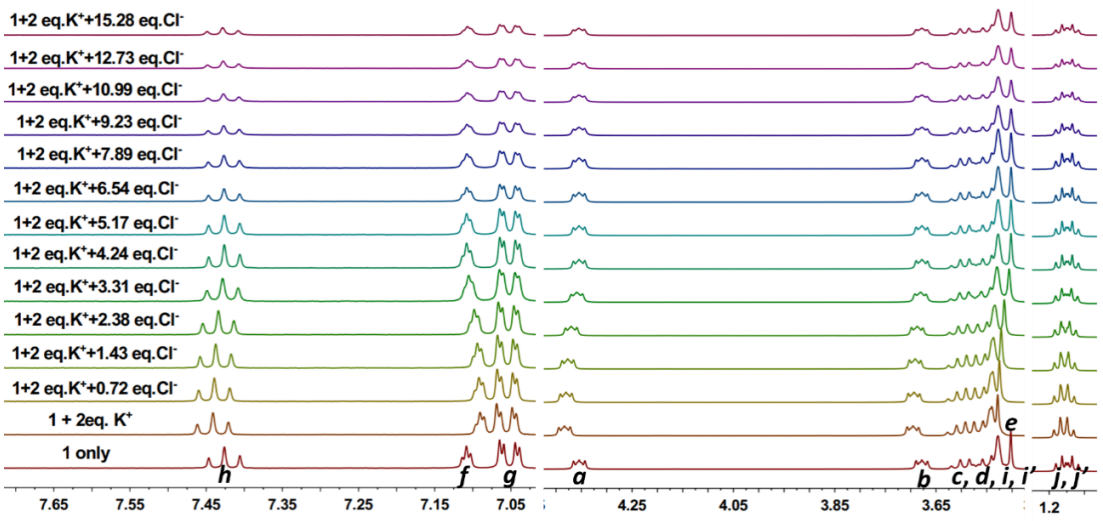


Figure S17. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and KPF_6 (2.10×10^{-2} M) with increasing equivalents of TBACl in CD_3CN.

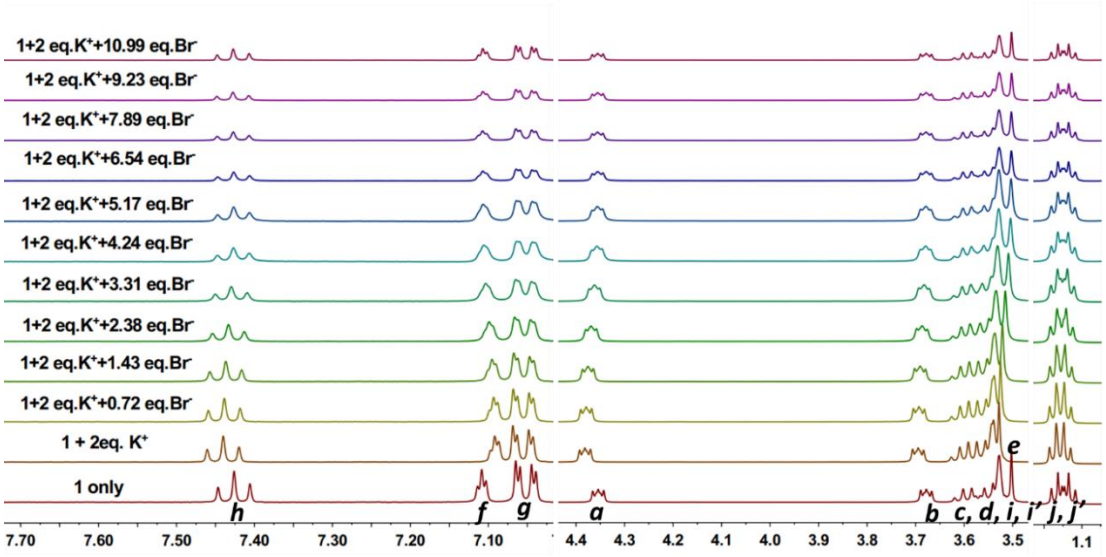


Figure S18. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and KPF_6 (2.10×10^{-2} M) with increasing equivalents of TBABr in CD_3CN.

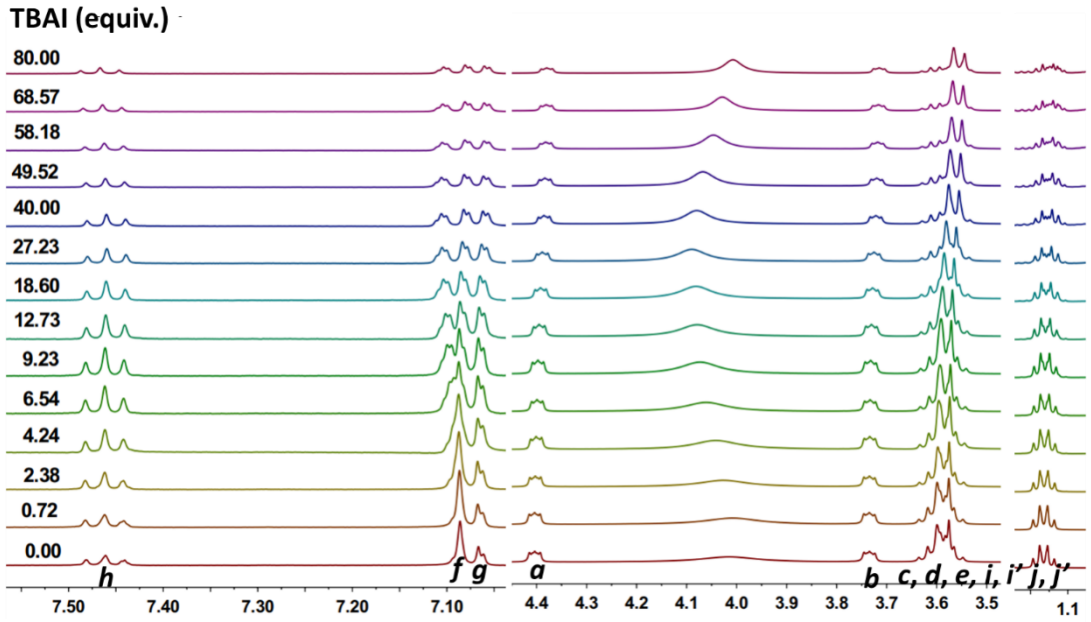


Figure S19. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $Mg(ClO_4)_2$ (2.10×10^{-2} M) with increasing equivalents of TBAI in CD_3CN.

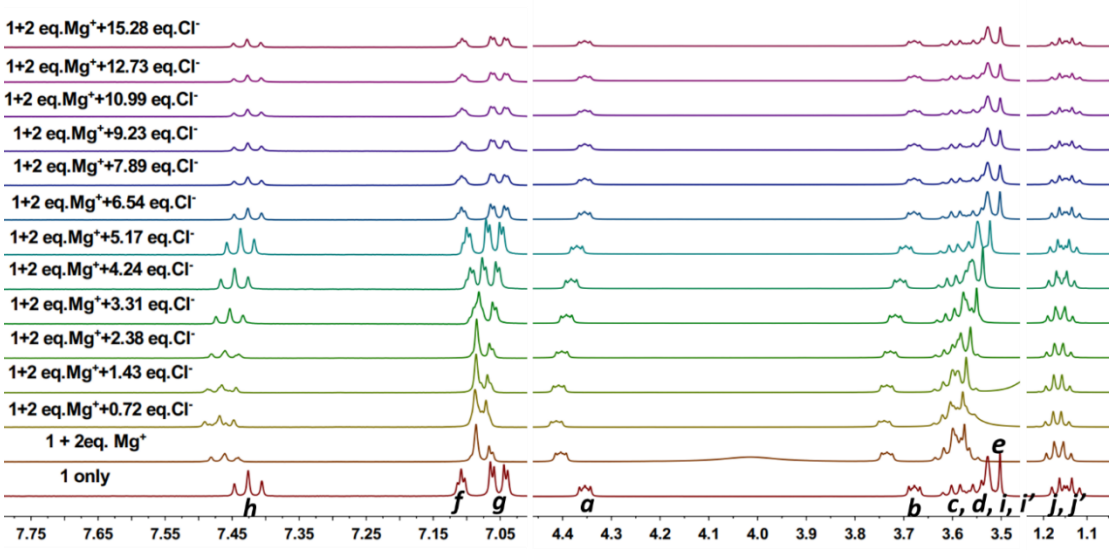


Figure S20. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $Mg(ClO_4)_2$ (2.10×10^{-2} M) with increasing equivalents of TBACl in CD_3CN.

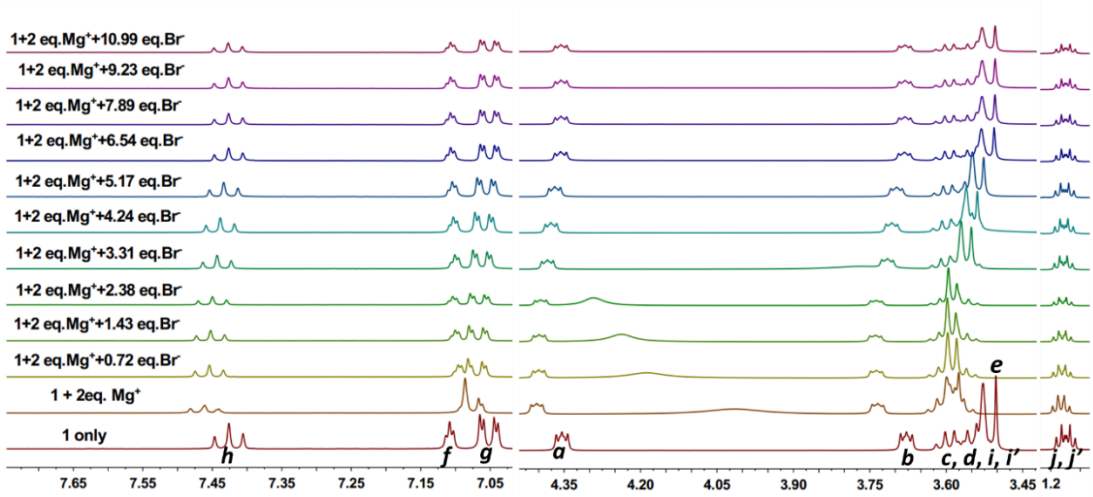


Figure S21. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $Mg(ClO_4)_2$ (2.10×10^{-2} M) with increasing equivalents of TBABr in CD_3CN.

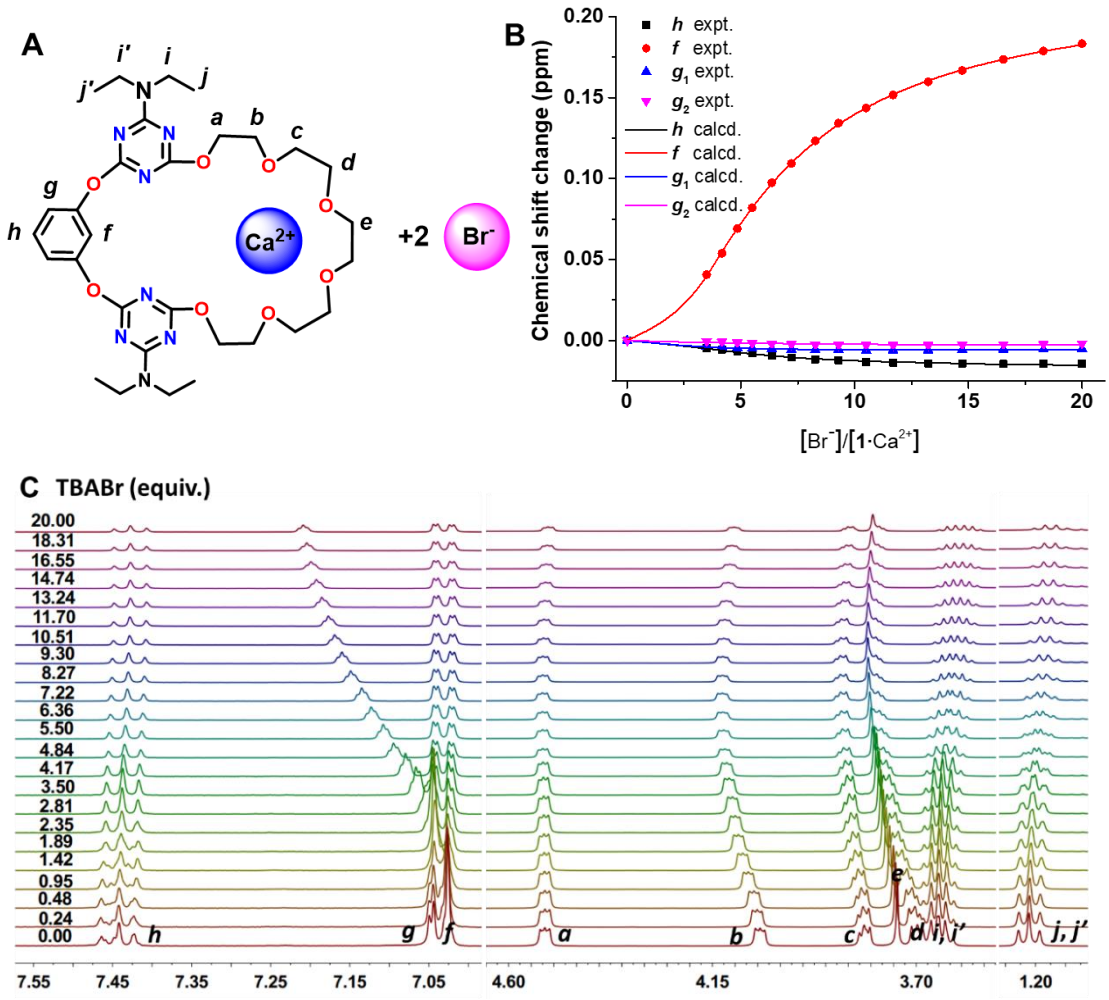


Figure S22. (a) A schematic binding mode of [**1**·Ca^{2+}·$2Br^{-}$] complex, (b) The fitting of the NMR titration data by *Bindfit v0.5* program, (c) ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $Ca(ClO_4)_2$ (2.10×10^{-2} M) with increasing equivalents of Bu_4NBr in CD_3CN.

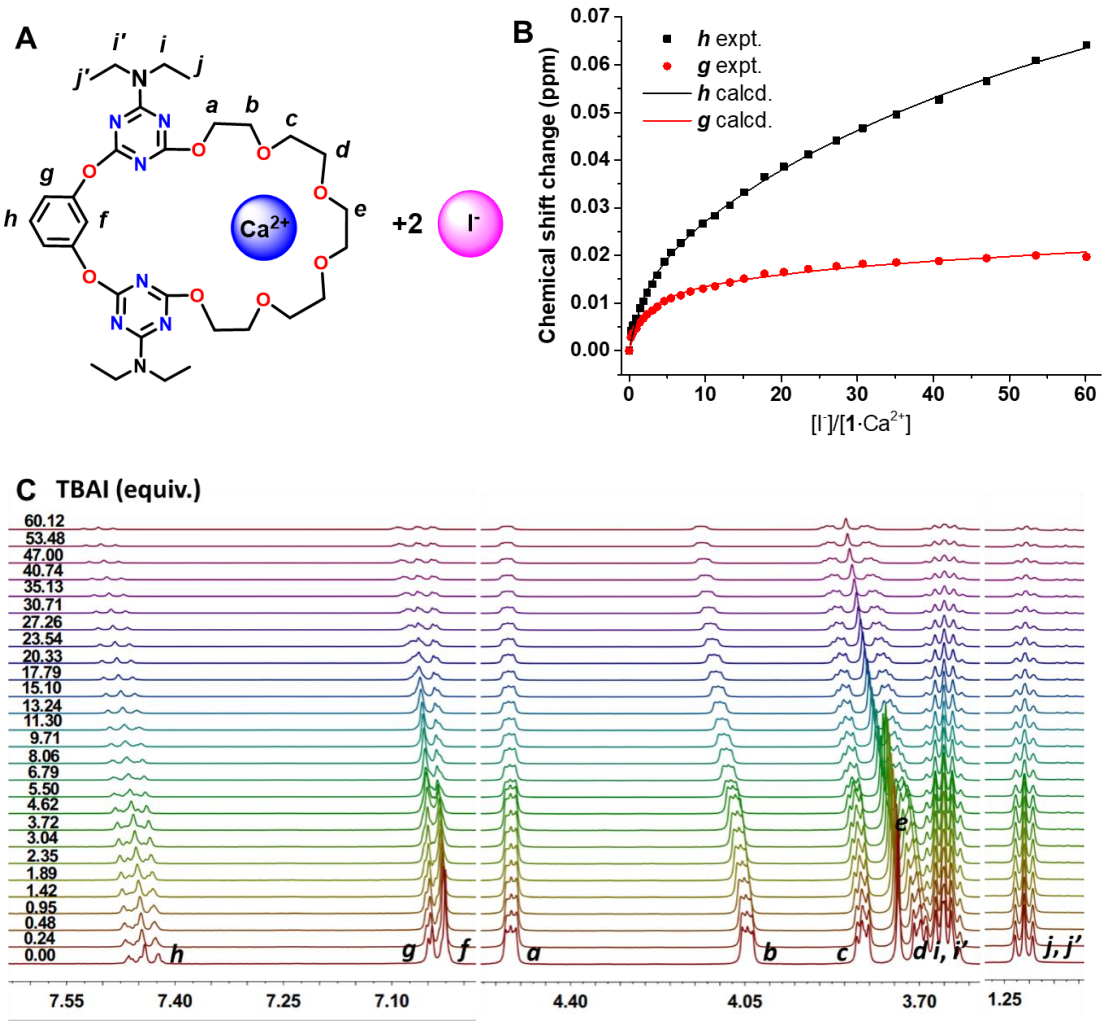


Figure S23. (a) A schematic binding mode of [**1**·Ca^{2+}·$2I^-$] complex, (b) The fitting of the NMR titration data by *Bindfit v0.5* program, (c) ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $Ca(ClO_4)_2$ (2.10×10^{-2} M) with increasing equivalents of Bu_4NI in CD_3CN.

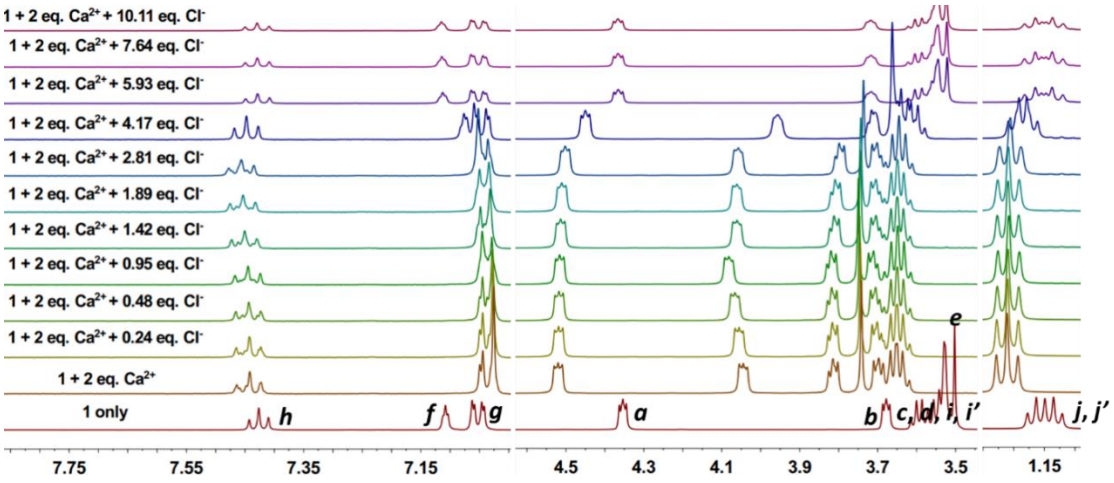
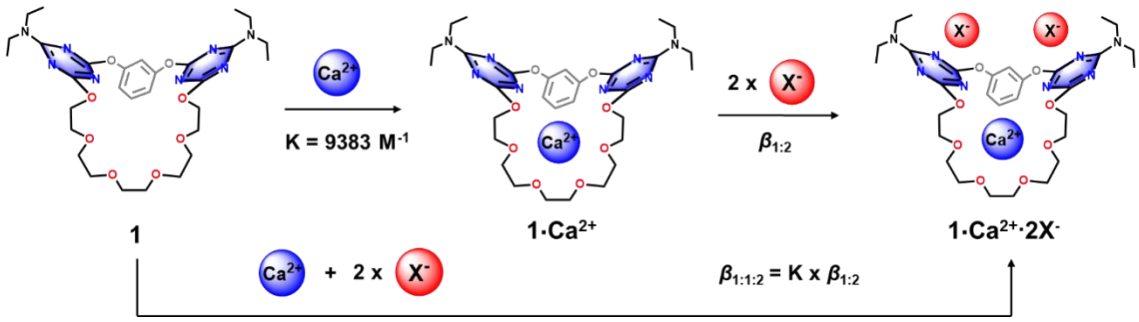


Figure S24. ^{1}H NMR titration of a mixture of **1** (1.05×10^{-2} M) and $Ca(ClO_4)_2$ (2.10×10^{-2} M) with increasing equivalents of Bu_4NCl in CD_3CN.

Table S2. Accumulative association constants determined by stepwise titrations. [a]



cation	β	Br^-	I^-
Ca^{2+}	$\beta_{1:2}$ (M^{-2})	1034	76
	$\beta_{1:1:2}$ (M^{-3})	9.70×10^6	7.18×10^5

[a] accumulative association constants were determined by ^{1}H NMR titration in CD_3CN (298K, 400 MHz), and fitted according to 1:2 binding model of *Bindfit v0.5* program.

3 Ion transport

3.1 General preparation for MCl ⊂ EYPC-LUVs[2-5]

The solution was produced during the EYPC (50 mg) was dissolved in the solution of MeOH/$CHCl_3$ (4 mL, v/v =1:1). The thin lipid film was obtained by evaporating this solution under reduced pressure on a rotary evaporator (40 °C) and then dried in vacuo for 48h. After hydration with 2.0 mL buffers (10 mM phosphate buffer, 500 mM NaCl or 500 mM KCl or 250 mM NaCl and 250 mM KCl or 166 mM $CaCl_2$, pH = 7.2) for 20 mins under the room temperature, the resulting suspension was subjected to 9 freeze-thaw cycles (with liquid N_2, 40 °C water bath) and 23 times extruded through a polycarbonate membrane (pore size 100 nm). Nonencapsulated salts were removed by dialysis.

3.2 General preparation for CF ⊂ EYPC-LUVs[2-4]

The solution was produced during the EYPC (25 mg) was dissolved in the solution of MeOH/$CHCl_3$ (2 mL, v/v =1:1). The thin lipid film was obtained by evaporating this solution under reduced pressure on a rotary evaporator (40 °C) and then dried in vacuo for 48h. After hydration with 1.0 mL buffers (10 mM phosphate buffer, 100 mM $NaNO_3$, 50.0 mM CF, pH = 7.4) for 20 mins under the room temperature, the resulting suspension was subjected to 5 freeze-thaw cycles (with liquid N_2, 50 °C water bath) and 21 times extruded through a polycarbonate membrane (pore size 100 nm). Extravesicular components were removed by size exclusion chromatography (Sephadex G-50). The corresponding buffer as mobile phase.

3.3 ISE assay[5]

A series of vesicles were suspended in an external solution (500 Mm $NaNO_3$ or 500 Mm KNO_3 or166 mM Na_2SO_4, buffered to pH 7.2 with 10 mM phosphate salts). The lipid concentration for each sample was 1 mM. An aliquot of the DMF solution of

a symporter, and the ion release from vesicles was monitored using an ion-selective electrode. The initial reading was considered as 0% release of an ion and the reading after the addition of 10% Triton X-100 to the lipid solution at 600 s was considered as 100% release. Transport experiments were performed on a ISE meter, and the chloride or potassium ion efflux was measured using a chloride or potassium ion selective electrode.

3.4 CF fluorescent assay[2-4]\

CF ⊂ EYPC-LUVs (50 μL) were added to gently stirred buffer (1950 μL, 100 mM $NaNO_3$, 50.0 mM CF, pH = 7.4) in a fluorescence cuvette (t = 0 s) at 25 °C. The time-dependent change in fluorescence intensity (I_t) was monitored at excitation wavelengths simultaneously (λ_{ex} = 369 nm, λ_{em} = 505 nm), during addition of acetone or carrier **1** in acetone (25 μL) at t = 50 s (I_0), and triton X-100 (25 μL, 10% in water) at t = 300 s (I_∞). The fluorescence intensity I_t was normalized to fractional intensity I_f according to equation:

$$I_f = (I_t - I_0) / (I_\infty - I_0) \qquad (1)$$

where I_0 is I_t at t = 50 s before addition of carrier, I_∞ is I_t at t = 300 s after addition of triton X-100.

Ion transport

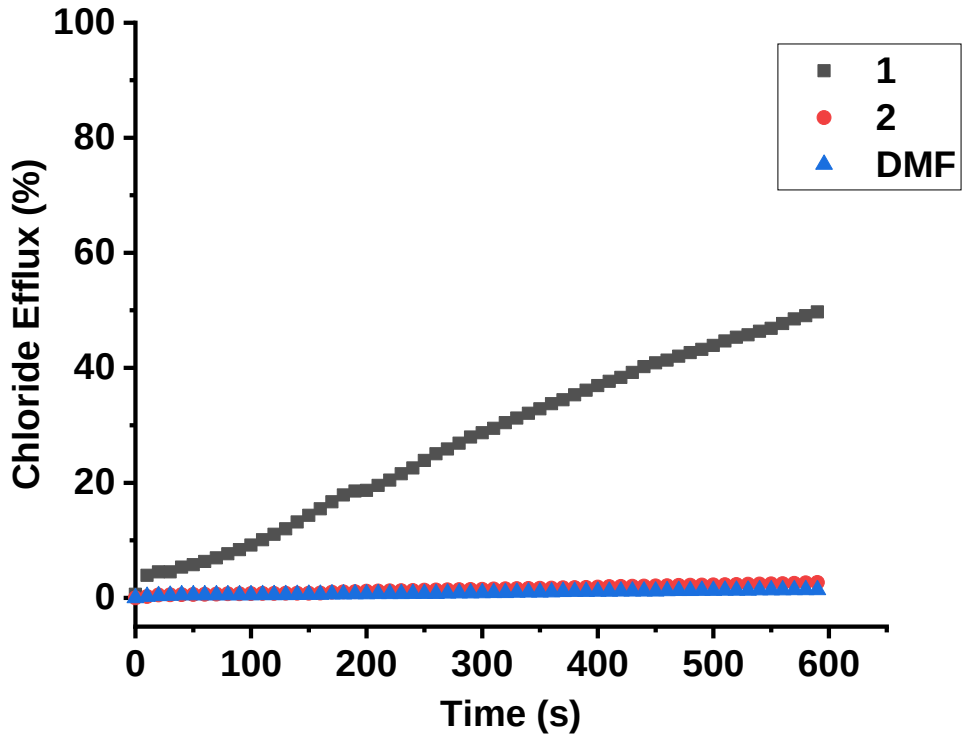
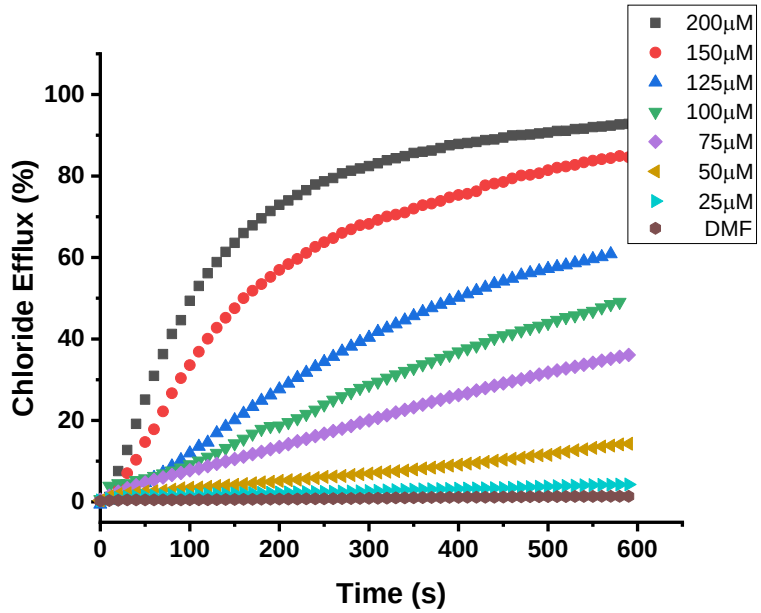


Figure S25. Chloride efflux facilitated by **1**, **2** and solvent (10 mol % of each compound to lipid) from EYPC vesicles (500 mM NaCl in 10 mM sodium phosphate buffer at pH = 7.2) to a phosphate buffer (500 mM $NaNO_3$ in 10 mM sodium phosphate buffer at pH = 7.2). Triton-100 was added to lyse the vesicles after 600 s, and chloride efflux was measured using a chloride selective electrode

(A)



(B)

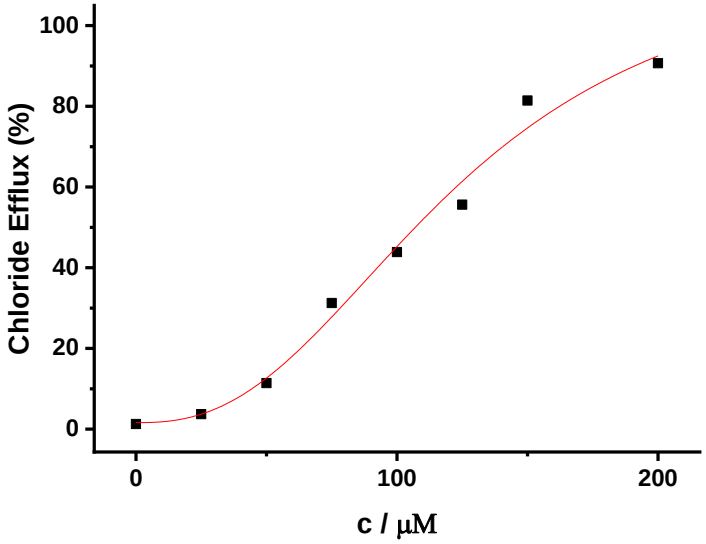


Figure S26. (A) Chloride efflux facilitated by **1** (in varied concentration) from EYPC vesicles (500 mM in 10 mM sodium phosphate buffer at pH = 7.2) to a phosphate buffer (500 mM $NaNO_3$ in 10 mM sodium phosphate buffer at pH = 7.2). Triton-100 was added to lyse the vesicles after 600 s, and chloride efflux was measured using a chloride selective electrode (B) Hill plot of the normalized intensities at 500 s. The EC_{50} is 119 μM.

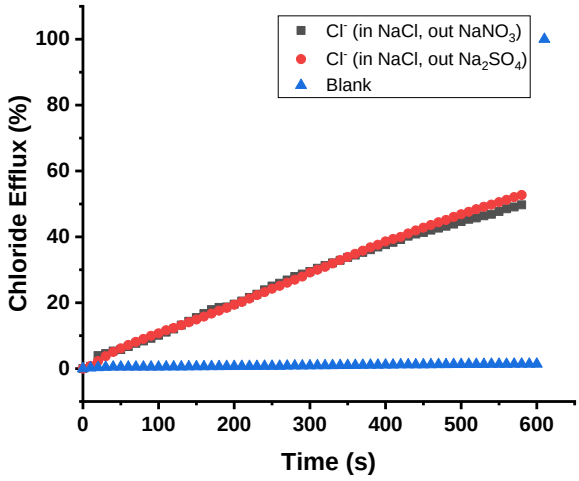


Figure S27. Chloride efflux facilitated by **1** and solvent (10 mol % of each compound to lipid) from EYPC vesicles (500 mM NaCl in 10 mM sodium phosphate buffer at pH = 7.2) to a phosphate buffer (500 mM $NaNO_3$ or 166 mM Na_2SO_4 in 10 mM phosphate buffer at pH = 7.2).

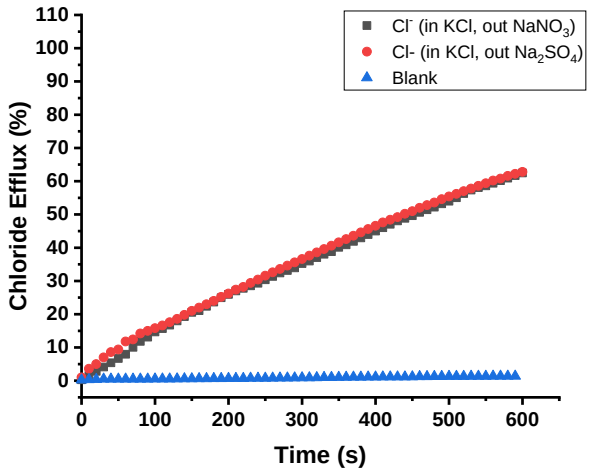


Figure S28. Chloride efflux facilitated by **1** and solvent (10 mol % of each compound to lipid) from EYPC vesicles (500 mM KCl in 10 mM potassium phosphate buffer at pH = 7.2) to a phosphate buffer (500 mM $NaNO_3$ or 166 mM Na_2SO_4 in 10 mM sodium phosphate buffer at pH = 7.2).

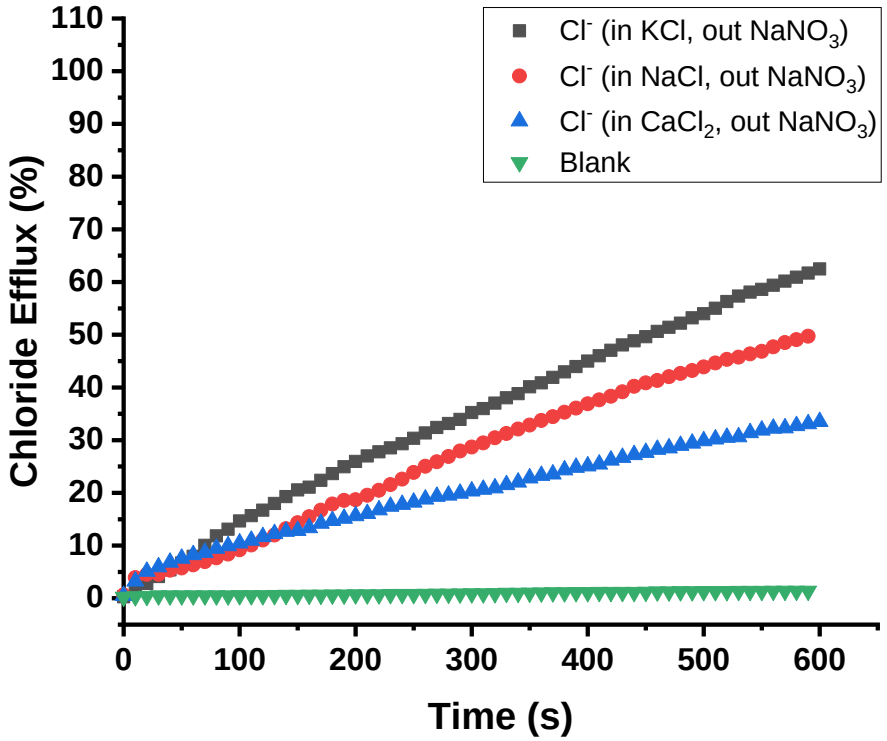


Figure S29. Chloride efflux facilitated by **1** and solvent (10 mol % of each compound to lipid) from EYPC vesicles (500 mM KCl, 500 mM NaCl or 166 mM $CaCl_2$ in 10 mM sodium phosphate buffer at pH = 7.2) to a phosphate buffer (500 mM $NaNO_3$ in 10 mM sodium phosphate buffer at pH = 7.2). Triton X-100 was added to lyse the vesicles after 600 s, and chloride efflux was measured using a chloride selective electrode

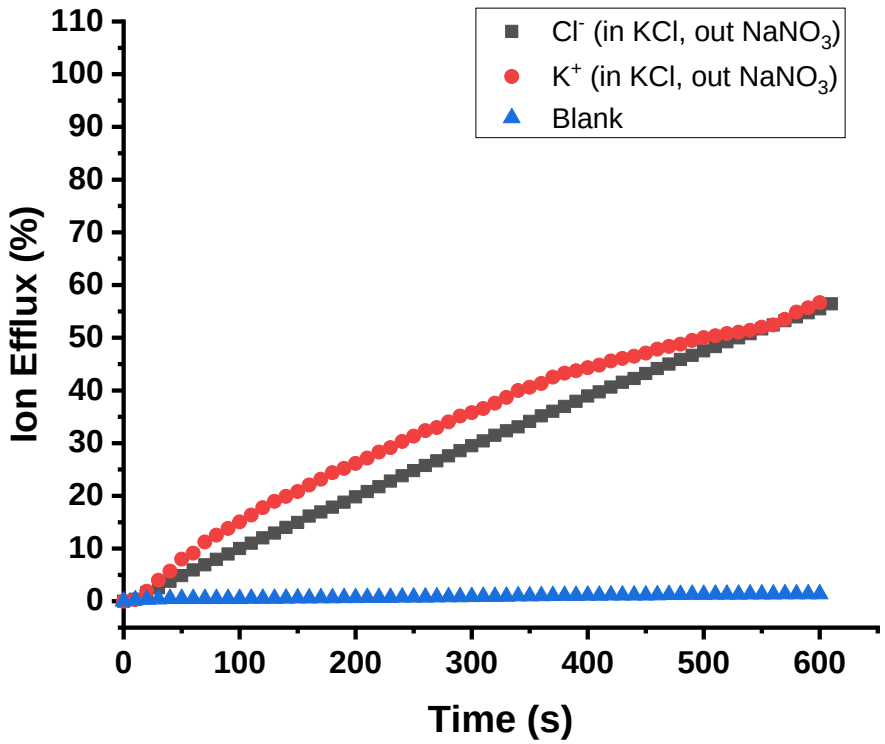


Figure S30. Chloride or Potassium efflux facilitated by **1** and solvent (10 mol % of each compound to lipid) from EYPC vesicles (500 mM KCl in 10 mM potassium phosphate buffer at pH = 7.2) to a phosphate buffer (500 mM $NaNO_3$ in 10 mM sodium phosphate buffer at pH = 7.2). Triton X-100 was added to lyse the vesicles after 600 s, and chloride efflux was measured using a chloride or Potassium selective electrode

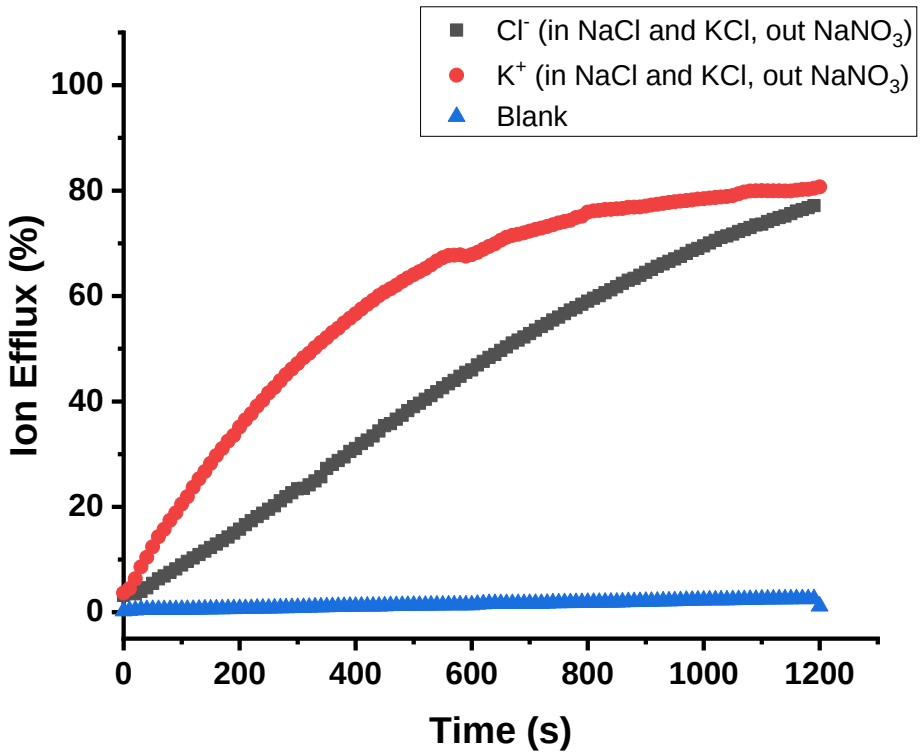


Figure S31. Chloride or Potassium efflux facilitated by **1** and solvent (10 mol % of each compound to lipid) from EYPC vesicles (250 mM KCl and 250 mM NaCl in 5 mM sodium phosphate and 5mM potassium phosphate buffer at pH = 7.2) to a phosphate buffer (500 mM $NaNO_3$ in 10 mM sodium phosphate buffer at pH = 7.2). Triton X-100 was added to lyse the vesicles after 1200 s, and chloride efflux was measured using a chloride or Potassium selective electrode

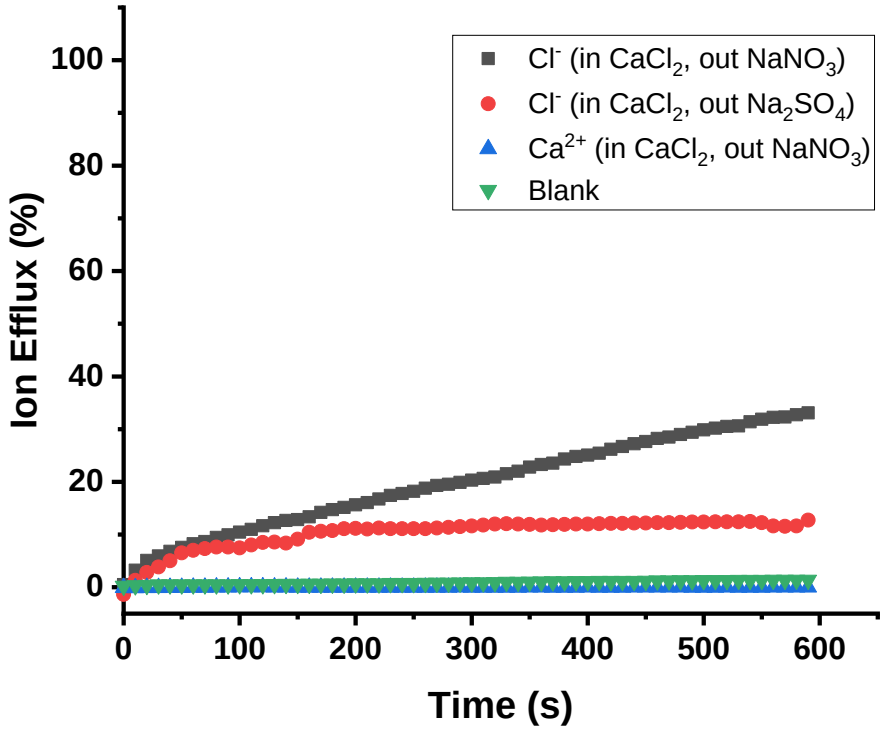


Figure S32. Chloride or Calcium efflux facilitated by **1** and solvent (10 mol % of each compound to lipid) from EYPC vesicles (500 mM KCl or 166 mM $CaCl_2$ in 10 mM sodium phosphate buffer at pH = 7.2) to a phosphate buffer (500 mM $NaNO_3$ or 166mM Na_2SO_4 in 10 mM sodium phosphate buffer at pH = 7.2). Triton X-100 was added to lyse the vesicles after 600 s, and chloride efflux was measured using a chloride or Calcium selective electrode

CF release experiment

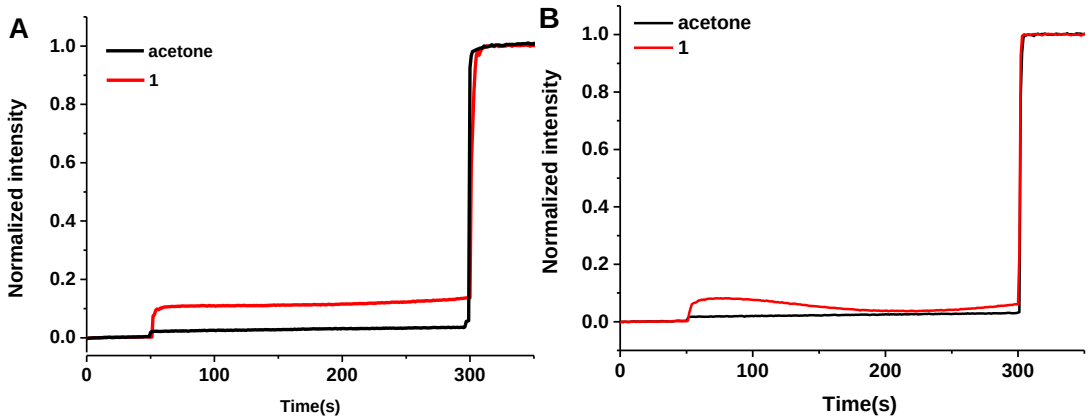


Figure S33. Normalized fluorescence intensity of CF (10 mM HEPES, 100 mM $NaNO_3$, pH = 7.4) ⊂ EYPC-LUVs with the addition of the transporter **1** (70 μM) or acetone, (A) the extravesicular salt is $CaCl_2$. (B) the extravesicular salt is NaCl。λ_{ex} = 492 nm, λ_{em} = 517 nm.

4. X-Ray diffraction data

Table S3. Crystal data and structure refinement for [**1**·Ca^{2+}·$2I^-$·$4H_2O$·$CHCl_3$]

CCDC number	2103643
Empirical formula	C31 H53 Ca Cl3 I2 N8 O12
Formula weight	1130.04
Temperature	173.15 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 21/n 1
Unit cell dimensions	a = 15.2822(5) Å α = 90° b = 20.3116(5) Å β = 117.084(5)°. c = 16.7995(6) Å γ = 90°.
Volume	4642.8(3) $Å^3$
Z	4
Density (calculated)	1.617 Mg/m^3
Absorption coefficient	1.699 m^{-1}
F(000)	2272
Crystal size	0.338 x 0.217 x 0.056 mm^3
Theta range for data collection	1.691 to 27.538°.
Index ranges	-19<=h<=17, -26<=k<=26, -20<=l<=21
Reflections collected	10593
Independent reflections	10593 [R(int) = ?]
Completeness to theta = 25.242°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.85477
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10593 / 0 / 521
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0338, wR2 = 0.0808
R indices (all data)	R1 = 0.0383, wR2 = 0.0828
Extinction coefficient	n/a
Largest diff. peak and hole	1.053 and -0.660 $e.Å^{-3}$

5. DFT optimization

For all free host molecules, free guest anions, and complexes, geometrical optimizations and energy calculations were carried out with the Gaussian16 suite of program using the X3LYP/6-31 G+(d) functional. The binding energy was calculated with BSSE correction.

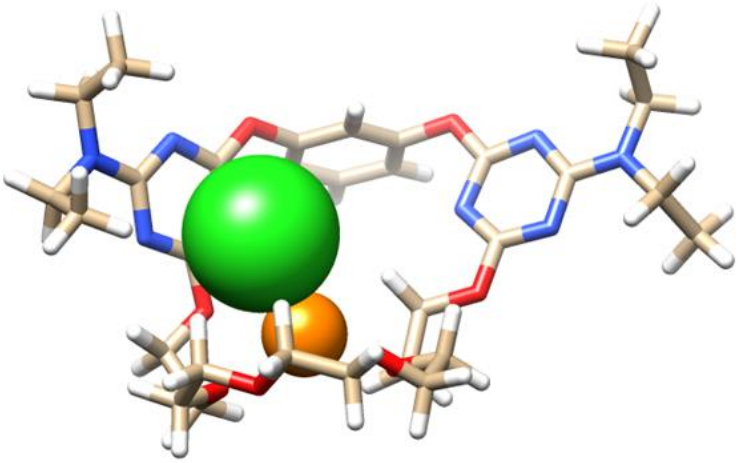


Figure S34. The DFT optimized structure of [**1**·Na^+·Cl^-] complex.

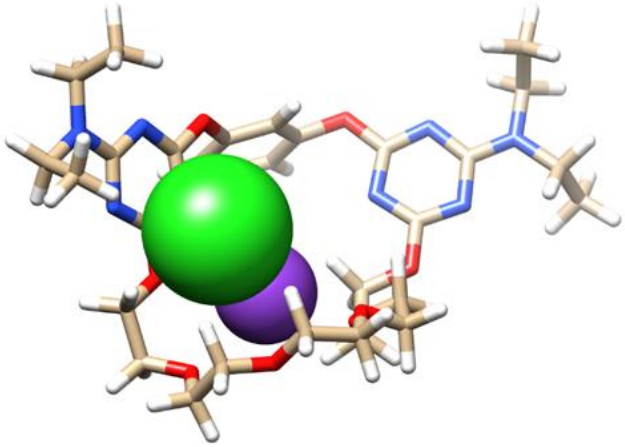


Figure S35. The DFT optimized structure of [**1**·K^+·Cl^-] complex.

Cartesian Coordinates (Angstrom) of the Optimized Complexes

[**1**·Ca^{2+}·$2Br^{-}$]

Atom	X	Y	Z
Br	-0.20560000	0.19795100	1.25544500
Br	-2.98484300	-3.58792700	-1.87583800
Ca	-1.58905800	-1.81369000	-0.13375200
O	4.83300100	2.36820200	-0.77899400
O	3.35505300	-1.97352000	-0.55257000
O	0.52429200	-3.18095600	-0.58075200
O	-0.91833300	-3.44460900	1.69066100
O	-3.20319100	-1.95825300	1.86753900
O	-3.68671600	-0.36353800	-0.30150000
O	-3.13870200	1.98261000	-1.92789700
O	0.44713200	3.93900600	0.08448800
O	-1.13925600	-1.05068900	-2.40433100
H	-1.64227800	-1.74293500	-2.88410500
N	6.04865200	0.84615500	0.33926000
N	5.26619700	-1.41203700	0.48554300
N	4.01472300	0.21670700	-0.72234100
N	-3.40592500	2.88383200	0.18175700
N	-1.50533300	3.95705000	1.14248200
N	-1.34244000	2.94907100	-1.00849600
C	4.95988700	1.08760500	-0.36893100
C	6.16296900	-0.43810500	0.75107100
C	4.23852500	-1.01271100	-0.25114600
C	2.24149200	-1.59754800	-1.38802000
H	2.61998200	-1.19647700	-2.33425200
H	1.65083400	-0.82275100	-0.89072200
C	1.41353800	-2.83988900	-1.64872700
H	0.76272100	-2.65496400	-2.50414700
H	2.06289700	-3.69615200	-1.87345200
C	1.11729700	-3.81582000	0.55227800
H	1.63596100	-3.07821800	1.17413800
H	1.83864200	-4.57554700	0.22436800
C	-0.00145900	-4.47557800	1.33222200
H	-0.50927900	-5.23632000	0.72411500
H	0.40672700	-4.94692300	2.23737200
C	-1.91603600	-3.79289700	2.64141300
H	-1.45412700	-4.25300500	3.52637700
H	-2.63293100	-4.50154900	2.20297900
C	-2.60683100	-2.50552000	3.04134600

H	-3.37998800	-2.71206700	3.79548300
H	-1.87424600	-1.79920500	3.45293100
C	-3.78709100	-0.66584700	2.06184100
H	-2.99071700	0.06922100	2.23460500
H	-4.46971200	-0.68676100	2.92343800
C	-4.57294400	-0.32891800	0.81416000
H	-5.37605400	-1.06341200	0.66061100
H	-5.00757100	0.67123600	0.92890200
C	-4.31112500	-0.09849700	-1.55931900
H	-5.29759800	-0.58025200	-1.59911900
H	-3.67834900	-0.57245300	-2.30908800
C	-4.44007300	1.39101800	-1.84146900
H	-4.89799400	1.52744500	-2.82643400
H	-5.03840700	1.91148400	-1.09290000
C	-2.62770100	2.62178400	-0.85962200
C	-2.79265000	3.58153900	1.16834600
C	-0.84907200	3.58212000	0.05313800
C	1.37673400	3.58783000	-0.88448500
C	1.22327100	3.88456200	-2.23908600
H	0.29515000	4.30657600	-2.60176500
C	2.28599800	3.62311200	-3.10383700
H	2.18087200	3.85271400	-4.16010300
C	3.48537000	3.08554100	-2.63323200
H	4.32152100	2.89217700	-3.29632900
C	3.60317700	2.80321400	-1.27733600
C	2.56024500	3.04781400	-0.39105500
H	2.65542400	2.83264900	0.66631900
C	-0.76765900	0.04690700	-3.24569700
H	-0.02061300	-0.26714300	-3.98483800
H	-0.34894800	0.81691800	-2.59749700
H	-1.64015100	0.46436200	-3.75740200
N	-3.53354900	3.93502900	2.25314900
N	7.25611400	-0.76619900	1.48729800
C	-4.93997300	3.60378200	2.36957900
H	-5.33245500	3.31461100	1.39696400
H	-5.09948800	2.78087200	3.08244300
H	-5.49111900	4.47790700	2.73656700
C	-2.93095400	4.57987100	3.40878200
H	-3.43030300	5.53611400	3.61052500
H	-3.03677900	3.94186400	4.29647800
H	-1.87554500	4.75332500	3.21253500
C	7.46750300	-2.11208900	1.98982700
H	7.50674700	-2.10528300	3.08730600
H	6.65312700	-2.75309800	1.66005900

H	8.42113400	-2.50854600	1.61700000
C	8.27103700	0.21264700	1.83714000
H	8.35028700	0.30095500	2.92878500
H	9.24847800	-0.10159700	1.44804900
H	8.00465300	1.17834900	1.41379100

[**2**·Ca^{2+}·$2Br^{-}$]

Atom	X	Y	Z
Br	0.03786600	0.27792200	-1.20205800
Br	3.30364700	-3.07898300	1.93001100
Ca	1.71011600	-1.54625100	0.13016400
Cl	-7.44359800	-1.80807800	-1.77133400
Cl	3.21380000	4.06618200	-2.88137700
O	-5.15323700	1.89122000	0.39493600
O	-3.19196900	-2.25749200	0.53967900
O	-0.23323400	-3.12327200	0.65111900
O	1.22138000	-3.30337700	-1.61916900
O	3.29345700	-1.54786900	-1.87617700
O	3.60339700	0.16370600	0.22459700
O	2.76635400	2.47748700	1.75463600
O	-0.95653300	3.93258500	-0.43210300
O	1.18748000	-0.78101600	2.39860400
H	1.78070800	-1.40729700	2.86977400
N	-6.17955400	0.14552900	-0.58485000
N	-5.14519200	-2.00103500	-0.54663200
N	-4.09661300	-0.14979800	0.52724200
N	2.95955300	3.18748900	-0.43306500
N	1.00088200	4.00840000	-1.49003900
N	0.89587600	3.20496100	0.75288700
C	-5.12401600	0.58291300	0.10686100
C	-6.10501000	-1.14857900	-0.86459100
C	-4.16195500	-1.43137500	0.16528900
C	-2.12594700	-1.70218400	1.34681600
H	-2.55801400	-1.28131700	2.26058000
H	-1.62501600	-0.90617200	0.78725300
C	-1.16813800	-2.82520500	1.69050200
H	-0.55558500	-2.51143600	2.53655000
H	-1.71805400	-3.73417800	1.96635400
C	-0.71959400	-3.93420700	-0.41972000
H	-1.37180100	-3.35028700	-1.07819700
H	-1.28973100	-4.78300500	-0.01981800
C	0.48650700	-4.44580900	-1.18004500
H	1.11867900	-5.07347400	-0.53768500

H	0.15237300	-5.03360000	-2.04607200
C	2.25093500	-3.55964900	-2.56853000
H	1.84527800	-4.11023600	-3.42856700
H	3.05360000	-4.15367200	-2.10940500
C	2.77268100	-2.21346900	-3.02524500
H	3.56646800	-2.35201300	-3.77283200
H	1.95899400	-1.62235300	-3.46550800
C	3.74607000	-0.21291500	-2.12969800
H	2.88427600	0.42994800	-2.34736500
H	4.43439400	-0.20414700	-2.98593200
C	4.48462400	0.26002000	-0.89723700
H	5.36369400	-0.37317100	-0.71554200
H	4.79905900	1.29887100	-1.04989300
C	4.19064000	0.53694900	1.47150600
H	5.23022700	0.18665800	1.52298500
H	3.62363500	0.00849800	2.23724500
C	4.13716300	2.03794600	1.71304400
H	4.54185600	2.25828000	2.70480100
H	4.68596400	2.60727200	0.96246500
C	2.20272400	2.96105800	0.64636800
C	2.27955000	3.71883400	-1.44177600
C	0.35254000	3.68665600	-0.35748600
C	-1.88021500	3.53155700	0.52979000
C	-1.81209500	3.92733700	1.86399900
H	-0.95811900	4.48517500	2.22574000
C	-2.86728100	3.59039900	2.71223000
H	-2.83172800	3.89577900	3.75343800
C	-3.97383200	2.88222300	2.24062800
H	-4.80653800	2.63133900	2.88844300
C	-4.00251900	2.50722500	0.90301400
C	-2.96679700	2.82085200	0.03188200
H	-2.99342700	2.53201100	-1.01166600
C	0.71987900	0.27619200	3.24059300
H	0.03625400	-0.10918800	4.00693900
H	0.19416200	0.98427000	2.59916900
H	1.55280000	0.79663100	3.72422300

[**1**·Na^+·Cl^-]

O	-3.81770000	-2.98124900	-0.13481900
O	-3.07560200	1.41698000	-1.19542100
O	-0.50973900	3.05792000	-1.30915300
O	0.48987100	4.38203400	0.88243700
O	3.20136200	4.25457600	0.38449900
O	3.46506200	2.38326700	-1.59778900
O	2.89754100	-0.52813700	-2.14831100
O	0.83290200	-3.95112700	0.04162600
N	-5.32781300	-1.43634700	0.48918900
N	-4.94417600	0.86601200	-0.06610500
N	-3.39032600	-0.80739200	-0.73891700
N	4.06746100	-1.66071400	-0.51509700
N	2.92014300	-3.41116500	0.63338900
N	1.81803300	-2.18918400	-1.09051900
C	-4.19149900	-1.69134900	-0.13588700
C	-5.67673000	-0.12671700	0.49367900
C	-3.82866700	0.44888700	-0.64639000
C	-1.83553400	1.02179700	-1.81687900
H	-2.04704300	0.35104800	-2.65669400
H	-1.21053200	0.48079700	-1.10038200
C	-1.14507200	2.27477600	-2.32010300
H	-0.33953100	1.97197700	-2.99675700
H	-1.85340900	2.90095800	-2.88154500
C	-1.38591800	3.80720400	-0.45526600
H	-1.80010500	3.15678700	0.32240900
H	-2.21887000	4.21728000	-1.04155900
C	-0.59458000	4.94244300	0.16181800
H	-0.21383500	5.61541900	-0.62203300
H	-1.25356300	5.51905700	0.83027200
C	1.39235700	5.32133600	1.45851300
H	0.99438400	5.69376500	2.41391200
H	1.53002000	6.17218700	0.77508200
C	2.71874200	4.62004200	1.67625500
H	3.42440400	5.30441600	2.17277000
H	2.58548800	3.72124100	2.29432900
C	4.34874300	3.40864000	0.39264700
H	4.14897800	2.52352800	1.01160100
H	5.22428600	3.94812000	0.78854300
C	4.62822500	3.00101400	-1.04060800
H	4.89303300	3.87503000	-1.65439400

H	5.47554500	2.30098900	-1.04090500
C	3.71519900	1.63230600	-2.78384700
H	4.51467800	2.11127400	-3.36808500
H	2.79585600	1.66573200	-3.37760600
C	4.08987400	0.18878600	-2.49418900
H	4.51375000	-0.27602400	-3.39451300
H	4.81717500	0.11607800	-1.68396400
C	2.95377800	-1.49055400	-1.20338900
C	3.99331000	-2.61809200	0.44319300
C	1.89726200	-3.13805500	-0.16083200
C	-0.32101800	-3.83230800	-0.73235300
C	-0.33696000	-4.25027400	-2.03904100
H	0.45662100	-4.55668500	-2.46216500
C	-1.54058200	-4.21342200	-2.72771600
H	-1.57116400	-4.50200700	-3.63206300
C	-2.69498200	-3.76455000	-2.11853300
H	-3.51831900	-3.74348100	-2.59186000
C	-2.62447300	-3.34841100	-0.80954500
C	-1.45840600	-3.37304700	-0.08686700
H	-1.43158400	-3.08700100	0.81828600
Na	1.53361900	2.48144200	-0.17090900
Cl	2.16174900	0.86830300	1.70506500
N	-6.83629600	0.21113000	1.10468000
N	5.06854500	-2.80211800	1.24578300
C	-7.69720700	-0.81090700	1.71003200
H	-8.72924000	-0.45284200	1.62031100
H	-7.60955100	-1.72676300	1.12331100
C	-7.26209200	1.61056200	1.19648000
H	-7.82338200	1.71400900	2.13207900
H	-6.37210100	2.23789200	1.27082200
C	-8.11929100	2.05579100	0.00855900
H	-7.54189000	2.00028100	-0.91945500
H	-9.01189100	1.42822600	-0.09876700
H	-8.44898000	3.09254600	0.14794400
C	-7.35427700	-1.09308500	3.17501000
H	-7.41637300	-0.18360300	3.78427900
H	-8.05404300	-1.82792500	3.59086600
H	-6.34154000	-1.49898600	3.25765400
C	5.02172500	-3.81127600	2.31236900
H	4.51551700	-4.69392400	1.91484800
H	6.05993900	-4.08822300	2.52675100
C	6.22143600	-1.90082300	1.15504200
H	7.09435000	-2.46458100	1.50277200
H	6.38064000	-1.66688700	0.10006600

C	6.06521400	-0.60304900	1.95710900
H	5.14122400	-0.08368500	1.68235900
H	6.03277000	-0.79620500	3.03428500
H	6.92033500	0.05734500	1.76049000
C	4.31536700	-3.35256800	3.59225600
H	4.82292100	-2.50047600	4.05534900
H	3.28290800	-3.06382600	3.37764600
H	4.30034100	-4.17611500	4.31711800

[**1**·K^+·Cl^-]

O	-3.94666400	-2.90353400	-0.58866000
O	-3.79853800	1.64930800	-1.14813300
O	-1.06095800	2.99617100	-0.85350700
O	0.35727500	3.94024200	1.37624000
O	2.98444700	4.37129500	0.45108900
O	3.74153600	2.84378700	-1.86999800
O	3.30032600	-0.06479400	-1.70898600
O	0.72258400	-3.42597600	-0.00469900
N	-5.60695900	-1.64287500	0.25457500
N	-5.52132700	0.73911400	-0.02340700
N	-3.81418700	-0.63922100	-0.94385300
N	4.32094900	-1.74162300	-0.51875000
N	2.91805200	-3.42593400	0.42647000
N	1.96620300	-1.68311600	-0.89079200
C	-4.47341900	-1.67933000	-0.42314400
C	-6.10780600	-0.39534400	0.43073500
C	-4.39708700	0.53459200	-0.69241700
C	-2.65288500	1.50671700	-2.01150800
H	-3.00935100	1.28647100	-3.02581600
H	-2.02674100	0.67736000	-1.67711800
C	-1.88092300	2.81264100	-2.00205000
H	-1.19182200	2.81019700	-2.85331900
H	-2.56760300	3.66354600	-2.11965600
C	-1.73204800	3.37011100	0.35654600
H	-1.84845300	2.48721200	0.99792000
H	-2.73264200	3.75918900	0.13484100
C	-0.93029500	4.44152300	1.06701500
H	-0.83929500	5.32847200	0.42042800
H	-1.46413800	4.73657200	1.98617200
C	1.22519300	4.91509400	1.94930500
H	0.96617500	5.07427200	3.00753600
H	1.10878100	5.86843900	1.41218700
C	2.65905700	4.44450400	1.83797400

H	3.30919500	5.17864500	2.34195000
H	2.80268100	3.46281600	2.31073700
C	4.33769300	4.00274700	0.20178500
H	4.56347600	3.05141700	0.70272900
H	5.01605700	4.78436600	0.58623900
C	4.52883000	3.89588500	-1.29902100
H	4.22579400	4.83569000	-1.77911600
H	5.59420300	3.72857700	-1.50580400
C	4.43339500	1.83326600	-2.59938200
H	5.42519300	2.19360000	-2.90514900
H	3.85236800	1.63591300	-3.50827600
C	4.60327900	0.54677500	-1.81331800
H	5.27734200	-0.13427300	-2.34523200
H	4.98896200	0.72352800	-0.80488000
C	3.21735400	-1.20977900	-1.00260400
C	4.12171300	-2.83262400	0.26059200
C	1.92064100	-2.81297200	-0.18506700
C	-0.33008400	-3.26903900	-0.89744900
C	-0.16482800	-3.45007800	-2.24736500
H	0.69839000	-3.59326600	-2.61756400
C	-1.28946500	-3.41751800	-3.05882100
H	-1.19447500	-3.54406700	-3.99531500
C	-2.54490500	-3.20492100	-2.52599500
H	-3.31348900	-3.18633900	-3.08393800
C	-2.65626100	-3.02054000	-1.16755700
C	-1.57361900	-3.05112800	-0.32530700
H	-1.67206600	-2.92738600	0.61108600
Cl	3.50224800	0.86617900	1.81112200
N	-7.27057100	-0.27629200	1.11104900
N	5.18850100	-3.37177000	0.88949000
C	-7.98141400	-1.46052300	1.60676700
H	-9.05084200	-1.22179900	1.58728800
H	-7.81023400	-2.28228900	0.90965800
C	-7.85589400	1.04018500	1.38387000
H	-8.38531500	0.96269100	2.34021800
H	-7.04473300	1.75940800	1.50918200
C	-8.80921300	1.51197400	0.28279800
H	-8.26907600	1.63793800	-0.66059200
H	-9.62439800	0.79614200	0.12465900
H	-9.25379100	2.47642400	0.55643800
C	-7.55043100	-1.87124800	3.01694700
H	-7.69439700	-1.05493800	3.73461600
H	-8.14271300	-2.72925300	3.35667600
H	-6.49483600	-2.15933200	3.02405200

C	5.01406800	-4.54496900	1.75655800
H	4.30893500	-5.22137700	1.26767000
H	5.98612600	-5.04795800	1.80060200
C	6.50001300	-2.71239700	0.82039000
H	7.25364200	-3.49711800	0.95055400
H	6.61578600	-2.30699400	-0.18684400
C	6.69497700	-1.59680100	1.85321100
H	5.90502800	-0.84243000	1.77350700
H	6.69043600	-1.98938500	2.87560100
H	7.66465500	-1.11014700	1.68601800
C	4.51573900	-4.22288000	3.16905800
H	5.21663800	-3.58070800	3.71128400
H	3.54617800	-3.71903400	3.12773500
H	4.39612300	-5.15449600	3.73610600
K	1.57721500	1.89869100	-0.21682500

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