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Supporting Information

Enhancing Selectivity of Cation Exchange with Anion Receptors

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I. Experimental details

A. Materials

Chemicals were obtained from Sigma Aldrich and Fisher Scientific as ACS regent grade +99.5% purity or better. The solvent used for the extraction experiments, 1,2-dichloroethane, was obtained from Sigma Aldrich at 99.9% ACS grade. The radiotracers ^{137}Cs and ^{22}Na used for spiking the solutions prior to the extraction experiments were obtained from Isotope Products Laboratories, Burbank, CA and PerkinElmer Isotopes, respectively. Both ^{137}Cs and ^{22}Na isotopes were obtained as the chloride form ^{137}CsCl and ^{22}NaCl.

B. Solvent extraction experiments using radiotracers

Solutions containing **1**, **2**, or **3c** or a combination of **1** or **2** with **3c** were prepared by dissolving the solids in 1,2-dichloroethane. The aqueous phases were prepared by dissolving solid CsOH monohydrate in MilliQ ultrapure water to make a stock solution at 0.01 M. The caustic aqueous solutions used in the extraction experiments were prepared from aqueous 10 M standardized NaOH solutions purchased from VWR international, this stock solution was used in conjunction with the CsOH stock solution to make the solutions used in the experiments. The concentration of NaOH was varied from experiment to experiment, the concentration of CsOH was constant for all experiments at 0.0001 M. For the liquid-liquid contacting experiments, equal volumes (0.600 mL) of each respective organic and aqueous phase were pipetted into small 2 mL polypropylene tubes. The solutions in the tubes were individually spiked with 0.005 mL of the radiotracer solution containing 50.0 μL of ^{137}Cs and 100.0 μL of ^{22}Na. After spiking, the tubes were sealed and placed on a rotating wheel (Glass-Col Laboratory rotator) set at 60 rpm in a temperature-controlled air-box set at 25 ± 0.2 °C. The samples were mixed on the rotating wheel for 1 h, then placed in a temperature-controlled centrifuge (Beckman Coulter Allegra 6R) and centrifuged at 3000 rpm for 5 min at 25 ± 0.2 °C. After centrifugation, aliquots of the separated phases were removed via pipette, and 0.300 mL of each phase were placed in individual sealable culture tubes for counting to determine the distribution ratios (D_{Cs} and D_{Na}). The samples were then placed on a Canberra Gamma Analyst Integrated Gamma Spectrometer. The Gamma Analyst is able to determine the D_{Na} and D_{Cs} greater than 2×10^{-6} under the conditions of our experiments. The uncertainty in the results was estimated at ±5% due to handling errors of the samples (pipetting and preparation).

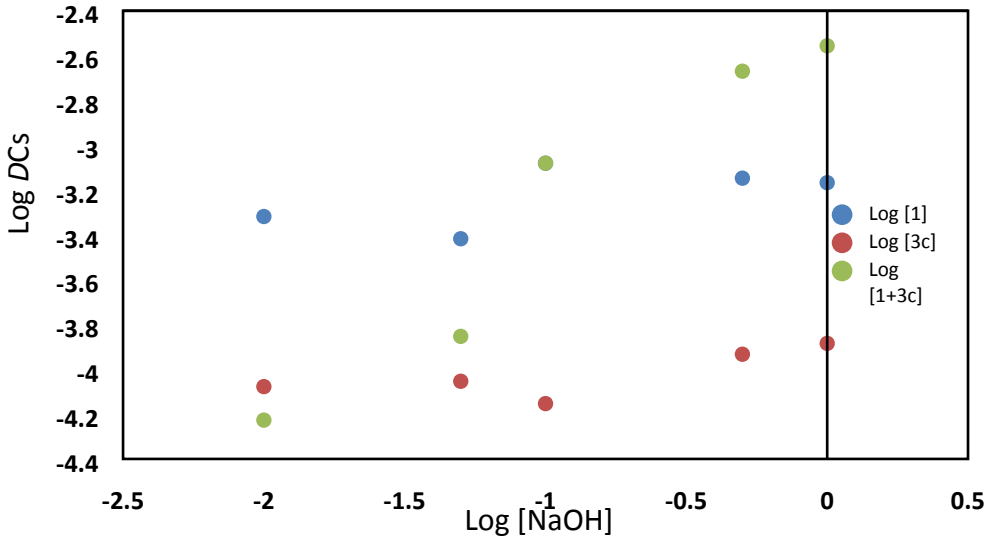

Figure S1. Log-log plot of continuous-variation experiments for cesium extraction from aqueous solution containing 1 M NaOH and 0.0001 M CsOH along with Cs-137 and Na-22 tracer into 1,2-DCE solutions of **3c** with **1** or **2**. The total

concentration of **1** or **2** and **3c** is 0.01 M. The points that are unfilled denote the presence of a third phase in the solutions. Sodium extraction was below detection.

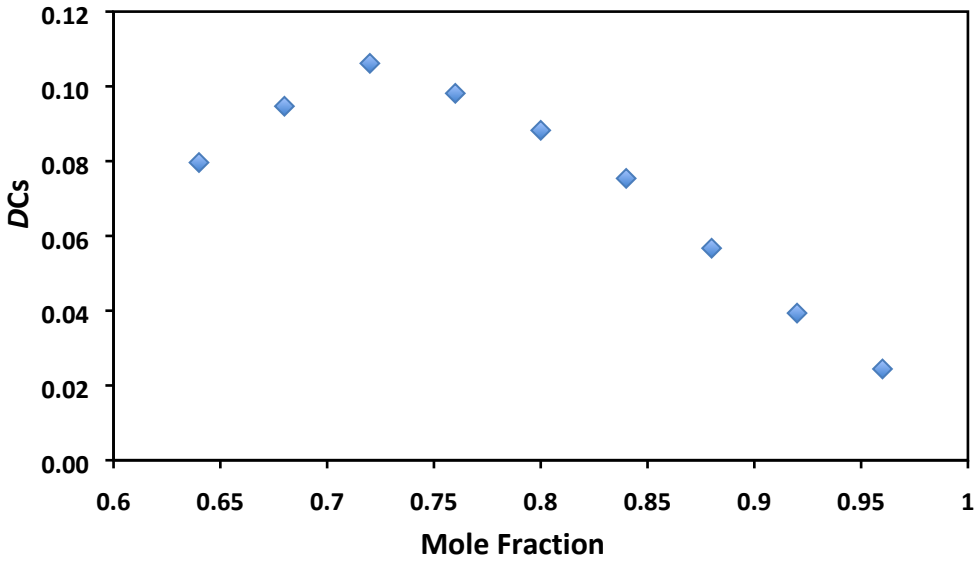

Figure S2. Continuous-variation experiment for cesium extraction from aqueous solution containing 1 M NaOH and 0.0001 M CsOH along with Cs-137 and Na-22 tracer into 1,2-DCE solutions of **3c** with **1** or **2**. The total concentration of **1** or **2** and **3c** is 0.025 M. The points that are unfilled denote the presence of a third phase in the solutions. Sodium extraction was below detection.

Continuous-variation experiments are shown in Figures S1 and S2. The data in Figure S2 are the same as shown in Figure 2 of the text except plotted on a log-log scale. As mentioned in the text, a rigorous interpretation of the continuous-variation experiments is not possible without precise knowledge of the aggregation behavior occurring in the system. However, some useful qualitative observations are possible for added insight. Based on prior experience with mass-action analysis of C4P systems, it is assumed that **1** and **3** are primarily in monomeric form at the concentrations used in this study ([**1**] + [**3**] = 10 or 25 mM).[1] However, salts of substituted phenols in organic solvents aggregate extensively.[2] At high concentrations (>0.5 M) in dry dichloromethane, phenol is a mixture of small aggregates and monomer.[3] Salts of the 4-alkylphenols also tend not to be soluble, and we in fact observed that **3c** under alkaline conditions produced a third phase in the absence of C4P. The third phase takes the form, as usual, as a heavy thin liquid layer at the interface between the bulk organic and aqueous phases. Accordingly, as the mole ratio increases in Figures S1, a third phase is present up to 0.3. Since mass balances for Cs are near 100% (i.e., total ^{137}Cs tracer activity for both bulk phases at equilibrium equals the starting aqueous ^{137}Cs tracer activity), no cesium resides in the third phase. This is interpreted as insolubility of the sodium phenolate salt and solubilization of the cesium phenolate by C4P.

Based on the structural and computational results, the simple supramolecular species $Cs^+(C4P)(PO^-)$ is postulated, where PO^- is a lipophilic phenolate anion. Because the Cs^+ within the C4P bowl is partly exposed to solvation interactions, as we saw earlier,[4] additional neutral POH molecules can possibly associate to form species like $Cs^+(C4P)(PO^-).n(POH)$. We may thus write a simple expectation for the equilibrium underlying the synergism:

$$Cs^+ + n\text{POH} + \text{C4P} + OH^- \rightleftharpoons Cs^+(C4P)(PO^-).(n-1)(POH) + H_2O \qquad \text{(S1)}$$

The quantitative interpretation of continuous-variation experiments in synergistic solvent extraction systems has been described in detail.[5] According to the simple stoichiometry given in 1, the maximum in

the curve would be found at $1/(n + 1)$.[5] The maxima observed at 0.5 in Figure S1 (and Figure 2 in the text) thus imply $n = 1$. However, at [**1**] + [**3**] = 25 mM, the maximum shifts to the higher value 0.72, as shown in Figure S2. This cannot be explained by $n > 1$, but is possibly an indication of the expected aggregation of POH. We might therefore postulate

$$Cs^+ + (1/y)(POH)_y + C4P + OH^- \rightleftharpoons Cs^+(C4P)(PO^-) + H_2O \quad \text{(S2)}$$

This stoichiometry leads to an expected maximum at $1/(1/y + 1)$. In this case, aggregation of POH in the form of dimers and trimers—realistic based on the behavior of phenol in dichloromethane[3]—reasonably explains the rightward shift of the maximum as seen in Figure S2. While this explanation fits known behavior and seems plausible if not likely, it is also possible that POH and C4P can interact to form adducts, which can further complicate the mass-action behavior.[5] Based on the available data, such an interaction cannot be ruled out.

C. Crystallization of 1 and 2 with 3a-b

1 and **2** were crystallized with **3a** and **3b** from 1,2-dichloroethane and methanol. 1,2-Dichloroethane was used to dissolve **1** and **2** at 0.025 M. The cesium salts of **3a** and **3b** were made by combining CsOH with the respective phenol at equal concentrations (0.1 M) in methanol, after mixing for 2 hrs. sodium sulfate was added to the mixture to remove water present in the methanol mixtures. Equal volumes of the calix[4]pyrrole (**1** or **2**) in 1,2-dichloroethane were combined with the cesium salt of either **3a** or **3b** in methanol in 20 mL glass scintillation vials. The vials were then sealed, and the solutions were allowed to set for 5 days after which small crystals had formed. The crystals were removed, and X-ray diffraction was performed to determine the structures.

II. Computational details

D. Electronic structure calculations

Electronic structure calculations were carried out using the Gaussian 16[6] Revision A.03 and NWChem 6.6[7] software packages. The def2TZVPP basis set was employed for hydrogen and main group elements,[8] while Cs was modeled using the 46MWB effective core potential (ECP46MWB)[9] and the associated basis set of comparable quality to the light elements. Due to large system size, geometry optimization for systems with receptor **2** was carried out with a smaller def2SVP basis set, followed by single-point energy calculations with the def2TZVPP basis set. Comparison of the performance of several DFT methods to reproduce the distortion energies for cation-π coordination complexes with 1,3-dimethylpyrrole at the CCSD(T)/def2TZVPP//MP2/def2TZVPP level (Figure S3)[7,10] indicates that M06-2X[11] provides the most accurate results for Cs^+, but somewhat overestimates the cation-π interaction energy for Na^+. The PBE-D3 density functional,[12,13] on the other hand, shows excellent agreement with benchmark CCSD(T) calculations for Na^+, but somewhat underestimates the cation-π interaction energy for Cs^+. PBE-D3 also accurately reproduces the X-ray structure in the solid state (Table S1). Based on these results, the M06-2X density functional was deemed sufficiently accurate for molecular calculations, while the PBE-D3 was considered for molecular dynamics simulations with periodic boundary conditions. Since optimization at the M06-2X level produced a distorted geometry for the C4P complex with Na^+ salt, in which Na^+ is coordinated to only two pyrrole rings (Figure 3d in the main text), the results were also checked with the PBE-D3 functional. In the latter case, a very similar geometry was obtained, with the energy difference between the global minimum and a more symmetric complex close to the one obtained with M06-2X (within 0.5 kcal/mol). Zero-point energies and thermal corrections were obtained based on the gas-phase optimized geometries at the M06-2X/def2SVP level. The standard Gibbs free energy of every species in the gas phase was calculated using the rigid rotor-harmonic oscillator approximation without scaling, except that vibrational frequencies lower than 60 cm^{-1} were raised to 60 cm^{-1}. This procedure is based on the so-called quasiharmonic approximation, which was first introduced by Truhlar

et al.[14] and serves as a way to correct for the well-known breakdown of the harmonic oscillator model for the free energies of low-frequency vibrational modes.

Solvent effects were described by explicitly including solvent molecules and including implicit solvent corrections for 1,2-DCE using the SMD[15] solvation model in Gaussian 16. By including solvent molecules into calculations, a thorough conformational search was performed to find the most stable complexes for metal ions and ion pairs with and without C4P. Two solvent molecules were included in complexes with C4P in order to complete the first coordination sphere around Cs^+ and Na^+ (Figure S4), as suggested by DFT-based molecular dynamics simulations (see section II. E). To account for the difference for the ion pair dissociation between Cs^+ and Na^+, we considered several model reactions with different number of solvent molecules, as summarized in Table S2. The results are not very sensitive to the choice of a particular model reaction, indicating that solvent effects were captured reasonably well. The electronic energies in the solvent reaction field were computed both as single point energies on gas-phase optimized geometries at the M06-2X/def2SVP level and after geometry optimization in the solvent reaction filed, in which case they were computed at the M06-2X/def2TZVPP level.

To elucidate the origin of enhanced extraction of Cs^+ with a more lipophilic anion receptor **2**, a total complexation free energy was broken down into three steps, as shown in Table S3. Each reactant and product must be represented in the most stable form. The most stable structure of the final complex with **2** is shown in Figure S5a, while the isomeric structure with a more symmetric arrangement of alkyl groups is shown in Figure S5b. A comparative analysis of Gibbs free energies indicates that most of the difference in binding between **1** and **2** is traced mainly to a stronger interaction of **2** with the 4-*t*-butylphenolate anion after the receptor adopts a binding cone conformation.

E. Ab initio molecular dynamics simulations

Born-Oppenheimer ab initio molecular dynamics (AIMD) simulations were performed using the Quickstep module of the CP2K 6.1 software,[16] where the valence electrons were treated explicitly at the PBE-D3 level. These simulations employed DZVP-MOLOPT basis[17] in conjunction with Goedecker-Teter-Hutter (GTH) pseudopotentials[18] and a 400 Ry cutoff for the auxiliary plane wave basis. The most stable structures of $Cs^+(1,2\text{-DCE})_2$**:1:3a** and $Na^+(1,2\text{-DCE})_2$**:1:3a** obtained from M06-2X/def2TZVPP calculations were placed in a periodic cubic box of 20.0 Å in size, containing additional 52 1,2-DCE molecules, which corresponds to a density of 1.245 and 1.222 g/cm^3, respectively. The initial configurations for MD simulations were generated by the MedeA Amorphous Cell Builder.[19] We chose the classically equilibrated configurations as the starting configurations for AIMD. Two systems were first pre-equilibrated with MedeA-LAMMPS[19,20] and the PCFF+[21,22] force field for 4 ns in an NVT ensemble at a temperature of 298.15 K. The DFT structures were kept frozen and only solvent molecules were allowed to move. The structures obtained from these pre-equilibration simulations were then subjected to 200 steps of unconstrained geometry optimization using the conjugate gradient method in CP2K, followed by AIMD simulations for at least 60 ps at 300 K using the Nosé-Hover thermostat[23] with a timestep of 0.5 fs. The last 50 ps of the AIMD trajectories were analyzed for the computation of structural parameters such as intermolecular distances, angles, and radial distribution functions (Figure S6). The 2D free energy surface ($W(d,\theta)$) as a function of the hydrogen bonding distance (d = donor-acceptor distance) and angle (θ = proton-donor-acceptor angle) was computed from the joint probability distribution of d and θ: $W(d, \theta)=-k_B T\ln[\Omega(d, \theta)/(d^2\, \delta d)(\sin\theta\, \delta\theta)]+C$, where k_B, T, $\Omega(d, \theta)$], and C are respectively Boltzmann constant, temperature, joint probability distribution function, and a constant to shift the global minimum to zero.[24] Movies of MD trajectories were prepared using VMD,[25] which are provided in a separate Microsoft PowerPoint file.

Table S1. Comparison of DFT M-ring centroid and M-oxygen of the deprotonated cation exchanger (CE^-) distances in the gas phase, 1,2-DCE solvent, and solid crystalline (both DFT and experimental) for ion-pair complexes with C4P[a]

Distance (Å)	M = Cs CE^- = **3b** Gas (M06-2X)	M = Cs CE^- = **3a** Liquid (PBE-D3)	M = Cs CE^- = **3a** Crystal (PBE-D3)	M = Cs CE^- = **3a** Crystal (X-Ray)	M = Na CE^- = **3b** Gas (M06-2X)	M = Na CE^- = **3a** Liquid (PBE-D3)
M^+-C_{12}	3.34	3.57±0.25	3.47	3.38	2.54	3.07±0.26
M^+-C_{34}	3.35	3.74±0.30	3.69	3.63	3.40	3.47±0.34
M^+-O_{Anion}	3.82	4.40±0.21	4.18	4.10	2.32	3.46±0.25
M^+-C_5			3.31	3.37		

[a]Two shortest and two longest M-ring centroid distances were averaged and denoted as C_{12} and C_{34}, respectively. The centroid for a fifth pyrrole ring of a different C4P molecule that interacts with the open face of Cs^+ in the crystalline solid is designated as C_5.

Table S2.The computed Gibbs free energies, $\Delta G_{r2,}$ for the listed reactions in 1,2-DCE solvent (kcal/mol)[a]. Slightly positive ΔG_{r2} means a greater tendency of Cs^+CE^- to dissociate in 1,2-DCE than Na^+CE^-

Reaction	Method I	Method II
$Cs^+(1,2\text{-DCE})_3 + Na^+{:}CE^-(1,2\text{-DCE})_3 \rightarrow Na^+(1,2\text{-DCE})_3 + Cs^+{:}CE^-(1,2\text{-DCE})_3$	-3.4	-3.9
$Cs^+(1,2\text{-DCE})_3 + Na^+{:}CE^-(1,2\text{-DCE})_2 \rightarrow Na^+(1,2\text{-DCE})_3 + Cs^+{:}CE^-(1,2\text{-DCE})_2$	-2.4	-3.2
$Cs^+(1,2\text{-DCE})_4 + Na^+{:}CE^-(1,2\text{-DCE})_2 \rightarrow Na^+(1,2\text{-DCE})_3 + Cs^+{:}CE^-(1,2\text{-DCE})_3$	-2.2	-3.2

[a]Solvent effects beyond explicit solvation were included employing single-point energy calculations (Method 1) and geometry optimization in the SMD solvent (Method II). The deprotonated cation exchanger (CE^-) in these reactions is 4-*t*-butylphenoxide.

Table S3. Comparison of the Gibbs free energy of binding of receptors **1** and **2** with Cs^+ and 4-*t*-butylphenolate ions in 1,2-DCE (kcal/mol)[a]

Reaction	C4P = **1**	C4P = **2**
Cs^+ + C4P-1,3-alternate → Cs^+:C4P-1,3-alternate	-1.15	-1.15
Cs^+:C4P-1,3-alternate → Cs^+:C4P-cone	1.02	0.43
Cs^+:C4P-cone + 4-t-butylPhO^- → Cs^+:C4P-cone: 4-t-butylPhO^-	-24.6	-28.2
Total:		
Cs^+ + C4P-1,3-alternate + 4-t-butylPhO^- → Cs^+:C4P-cone: 4-t-butylPhO^-	-24.7	-28.9

[a]Solvent effects were included as single point energy corrections obtained using the SMD model.

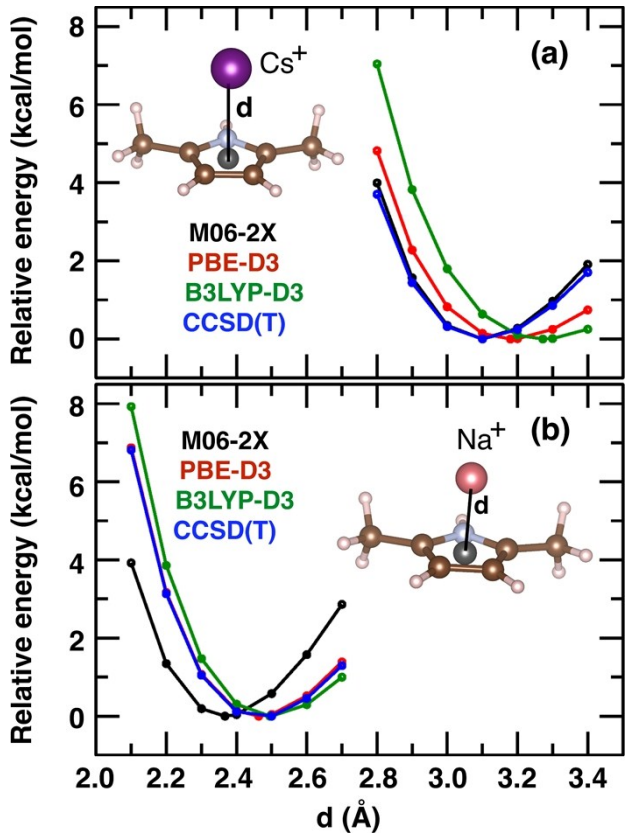

Figure S3. Potential energy surfaces for Cs^+ and Na^+ displacement along the line defined by the ion position in the global minimum and the centroid of the ring in 1,3-dimethylpyrrole. All calculations were performed with the def2TZVPP basis set. This includes the use of all-electron basis set for Na and the ECP46 MWB pseudopotential for Cs. Single-point calculations at the CCSD(T) level were performed on MP2/def2TZVPP geometries.

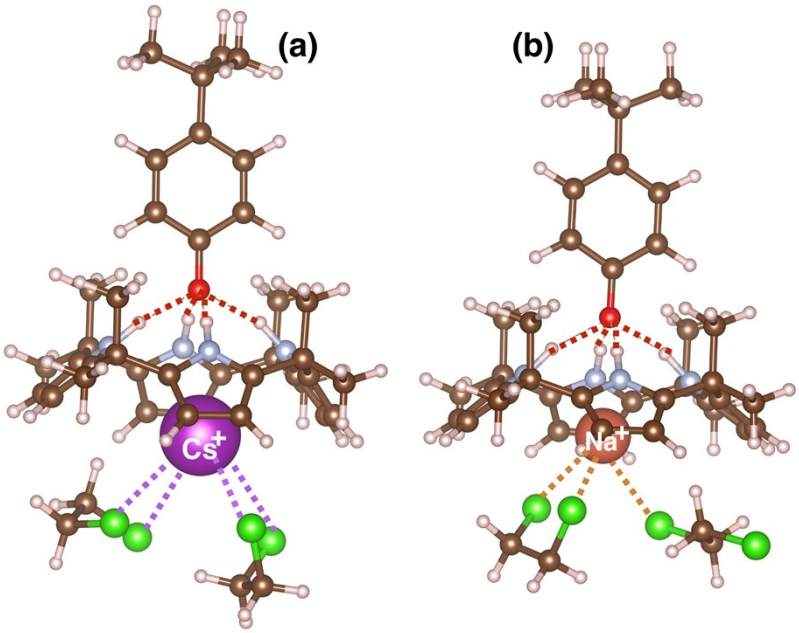

Figure S4. The most stable ion-pair cesium- and sodium-4-t-butylphenolate complexes with C4P, (a) $Cs^+(1,2\text{-DCE})_2$:**1**:**3b** and (b) $Na^+(1,2\text{-DCE})_2$:**1**:**3b**, with two explicit 1,2-DCE solvent molecules. Calculations were performed at the M06-2X/def2TZVPP level, with solvent corrections obtained using the SMD solvation model.

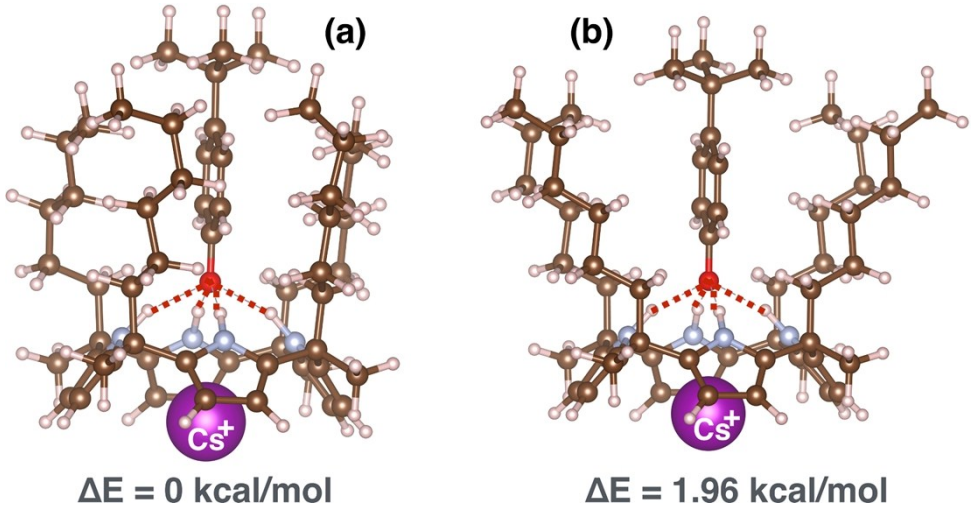

Figure S5. Relative free energies of isomeric complexes with a different arrangement of alkyl groups in lipophilic C4P around the 4-t-bytulphenolate anion. The initial complexes were taken from (a) Cs^+:**2**:**3a** and (b) Cs^+:**2**:**3b** crystal structures.

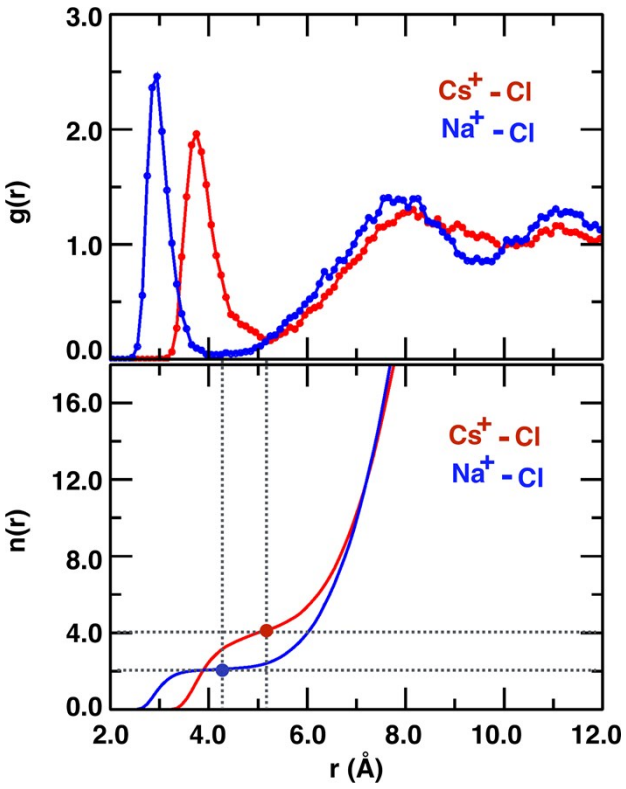

Figure S6. Radial distribution functions of chlorine atoms of solvent around Cs^+ and Na^+ (g(r), upper panel) and their integration (n(r), lower panel) for Cs^+:**1**:**3a** and Na^+:**1**:**3a** complexes in 1,2-DCE obtained from DFT-based molecular dynamics simulations.

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Cartesian coordinates and electronic energies of the studied complexes obtained at the M06-2X/def2TZVPP/ECP46MWB(Cs) level for receptor 1 and M06-2X/def2TZVPP/ECP46MWB(Cs)// M06-2X/def2SVP/ECP46MWB(Cs) level for receptor 2.

Cs^+**1**:**3b**; E(RM062X) = -1791.95428185 A.U.

Cs	2.8141	-0.0116	0.0002
N	0.5946	-0.0014	2.4030
H	-0.1727	0.0034	1.7245
C	1.2196	-1.1303	2.8684
N	0.5644	-2.3926	-0.0010
H	-0.1804	-1.6839	-0.0008
C	2.2882	-0.7235	3.6301
H	2.9637	-1.3685	4.1659
N	0.5948	0.0008	-2.4031
H	-0.1726	0.0051	-1.7247
C	2.2969	0.6990	3.6306
H	2.9801	1.3354	4.1670
N	0.5937	2.3927	0.0010
H	-0.1598	1.6932	0.0007
C	1.2333	1.1195	2.8692
C	0.7607	2.5110	2.5202
C	1.3628	3.5057	3.5133
H	2.4517	3.4868	3.4879
H	1.0414	3.2588	4.5245
H	1.0337	4.5158	3.2713
C	-0.7706	2.5824	2.6089
H	-1.1114	3.5837	2.3438
H	-1.0926	2.3565	3.6256
H	-1.2590	1.8738	1.9395
C	1.2229	2.8664	1.1261
C	2.2783	3.6421	0.7125
H	2.9516	4.1860	1.3529
C	2.2784	3.6428	-0.7093
H	2.9516	4.1873	-1.3492
C	1.2230	2.8673	-1.1237
C	0.7609	2.5133	-2.5181
C	-0.7704	2.5847	-2.6068
H	-1.0925	2.3597	-3.6237
H	-1.1112	3.5857	-2.3408
H	-1.2588	1.8755	-1.9380
C	1.3630	3.5089	-3.5103
H	2.4518	3.4899	-3.4849
H	1.0339	4.5187	-3.2674
H	1.0415	3.2629	-4.5217
C	1.2335	1.1221	-2.8683
C	2.2973	0.7023	-3.6299
H	2.9805	1.3391	-4.1655
C	2.2887	-0.7202	-3.6304
H	2.9642	-1.3648	-4.1667
C	1.2200	-1.1277	-2.8692
C	0.7302	-2.5132	-2.5201
C	1.3200	-3.5154	-3.5131
H	1.0009	-3.2651	-4.5243
H	0.9793	-4.5214	-3.2706
H	2.4090	-3.5092	-3.4883
C	-0.8020	-2.5657	-2.6088
H	-1.2813	-1.8512	-1.9392
H	-1.1551	-3.5628	-2.3441
H	-1.1213	-2.3354	-3.6254
C	1.1879	-2.8740	-1.1261
C	2.2335	-3.6629	-0.7123

H	2.9001	-4.2150	-1.3527
C	2.2334	-3.6635	0.7094
H	2.8999	-4.2162	1.3494
C	1.1877	-2.8750	1.1237
C	0.7298	-2.5155	2.5179
C	1.3194	-3.5185	3.5102
H	2.4084	-3.5123	3.4855
H	0.9787	-4.5243	3.2666
H	1.0002	-3.2692	4.5215
C	-0.8024	-2.5680	2.6063
H	-1.1219	-2.3386	3.6230
H	-1.1554	-3.5649	2.3406
H	-1.2816	-1.8530	1.9372
O	-1.0079	0.0097	-0.0000
C	-2.3400	0.0241	-0.0001
C	-3.0700	1.2210	0.0007
H	-2.5325	2.1629	0.0014
C	-4.4591	1.2263	0.0008
H	-4.9620	2.1838	0.0016
C	-5.2004	0.0487	-0.0000
C	-4.4741	-1.1444	-0.0010
H	-5.0008	-2.0917	-0.0018
C	-3.0913	-1.1656	-0.0010
H	-2.5678	-2.1154	-0.0017
C	-6.7275	0.0155	-0.0001
C	-7.2270	-0.7231	1.2493
C	-7.2269	-0.7192	-1.2518
H	-6.8923	-0.2077	-2.1553
H	-6.8544	-1.7430	-1.2875
H	-8.3183	-0.7567	-1.2603
H	-6.8552	-1.7473	1.2814
H	-8.3185	-0.7600	1.2579
H	-6.8919	-0.2150	2.1545
C	-7.3329	1.4191	0.0021
H	-7.0354	1.9849	-0.8821
H	-8.4214	1.3456	0.0024
H	-7.0348	1.9823	0.8878

$Cs(1,2\text{-DCE})_2^+$**1**:**3b**; E(RM062X) = -3790.00303569 A.U.

N	-0.6374	0.7909	2.2659
H	-1.4107	0.5333	1.6466
C	0.0456	-0.0887	3.0652
N	-0.6112	-2.3061	0.8641
H	-1.3583	-1.6438	0.6193
C	1.1309	0.5812	3.5776
H	1.8578	0.1798	4.2631
N	-0.5750	-0.8536	-2.1960
H	-1.3503	-0.6344	-1.5646
C	1.0850	1.9127	3.0796
H	1.7636	2.7106	3.3319
N	-0.6342	2.1691	-0.7738
H	-1.2966	1.4225	-0.5151
C	-0.0257	2.0179	2.2754
C	-0.5973	3.2029	1.5288
C	-0.0539	4.4893	2.1518
H	1.0339	4.5355	2.0891
H	-0.3358	4.5395	3.2025
H	-0.4623	5.3566	1.6334
C	-2.1293	3.2041	1.6460
H	-2.5387	4.0624	1.1126
H	-2.4239	3.2640	2.6942

H	-2.5758	2.3046	1.2222
C	-0.1881	3.1494	0.0764
C	0.6508	3.9674	-0.6408
H	1.1414	4.8503	-0.2637
C	0.7160	3.4582	-1.9667
H	1.2688	3.8763	-2.7910
C	-0.0940	2.3509	-2.0235
C	-0.4479	1.4638	-3.1938
C	-1.9751	1.4265	-3.3692
H	-2.2352	0.8224	-4.2389
H	-2.3562	2.4383	-3.5118
H	-2.4768	0.9986	-2.5010
C	0.1818	2.0463	-4.4596
H	1.2670	2.1032	-4.3720
H	-0.2021	3.0506	-4.6368
H	-0.0628	1.4197	-5.3162
C	0.0693	0.0571	-2.9964
C	1.1404	-0.5879	-3.5675
H	1.8311	-0.1613	-4.2749
C	1.1282	-1.9322	-3.1049
H	1.8054	-2.7167	-3.3970
C	0.0541	-2.0703	-2.2591
C	-0.4261	-3.2655	-1.4674
C	0.1905	-4.5314	-2.0636
H	-0.1197	-4.6417	-3.1022
H	-0.1359	-5.4046	-1.4996
H	1.2793	-4.4928	-2.0341
C	-1.9562	-3.3659	-1.5414
H	-2.4494	-2.4772	-1.1461
H	-2.2999	-4.2251	-0.9644
H	-2.2696	-3.4873	-2.5784
C	0.0232	-3.1341	-0.0300
C	1.0801	-3.7166	0.6260
H	1.7662	-4.4338	0.2090
C	1.0790	-3.2262	1.9600
H	1.7606	-3.5061	2.7453
C	0.0224	-2.3570	2.0815
C	-0.4173	-1.5161	3.2574
C	0.2170	-2.0736	4.5323
H	1.3050	-2.0580	4.4756
H	-0.1018	-3.1042	4.6856
H	-0.0877	-1.4750	5.3901
C	-1.9457	-1.5558	3.3993
H	-2.2532	-0.9709	4.2665
H	-2.2784	-2.5858	3.5306
H	-2.4543	-1.1488	2.5247
O	-2.2119	-0.0790	0.0363
C	-3.5430	-0.0678	0.0070
C	-4.2670	1.0440	-0.4452
H	-3.7236	1.9205	-0.7797
C	-5.6557	1.0460	-0.4705
H	-6.1536	1.9360	-0.8309
C	-6.4019	-0.0509	-0.0499
C	-5.6805	-1.1593	0.4007
H	-6.2109	-2.0421	0.7388
C	-4.2980	-1.1762	0.4316
H	-3.7769	-2.0582	0.7877
C	-7.9289	-0.0840	-0.0618
C	-8.4502	-0.3020	1.3654
C	-8.4134	-1.2350	-0.9541
H	-8.0561	-1.1042	-1.9764

H -8.0523 -2.1978 -0.5923
H -9.5050 -1.2688 -0.9706
H -8.0803 -1.2378 1.7845
H -9.5418 -0.3375 1.3705
H -8.1282 0.5101 2.0187
C -8.5271 1.2173 -0.5947
H -8.2129 1.4105 -1.6215
H -9.6160 1.1494 -0.5844
H -8.2388 2.0712 0.0202
Cs 1.6843 -0.1805 0.0906
Cl 4.4770 -1.8669 1.5437
Cl 4.1328 -2.0138 -1.7828
C 5.6711 -2.1600 -0.8921
C 5.6814 -1.3072 0.3509
H 6.4601 -1.8301 -1.5643
H 5.8058 -3.2115 -0.6556
H 6.6552 -1.3696 0.8317
H 5.4514 -0.2691 0.1228
Cl 4.0730 1.7501 -1.6490
Cl 4.4432 1.8143 1.6612
C 3.5590 3.0427 0.7167
C 4.1361 3.2379 -0.6624
H 3.6276 3.9783 1.2695
H 2.5142 2.7428 0.6776
H 3.5440 3.9828 -1.1897
H 5.1774 3.5439 -0.6213

$Cs(1,2\text{-DCE})_2^+$**2**:**3b**; E(RM062X) = -2578.12423044 A.U.
Cs -3.8297 -0.0065 1.1590
N -2.8094 0.2573 -1.9404
H -1.8311 0.1934 -1.6034
C -3.5373 1.4216 -2.0300
N -1.7416 2.4037 0.4315
H -1.0755 1.7257 0.0334
C -4.8299 1.0792 -2.3756
H -5.6473 1.7710 -2.5559
N -0.7867 -0.2130 2.3334
H -0.4344 -0.1361 1.3620
C -4.8763 -0.3382 -2.5064
H -5.7356 -0.9308 -2.8059
N -1.8799 -2.3672 -0.0162
H -1.1609 -1.6773 -0.2821
C -3.6108 -0.8210 -2.2368
C -3.0989 -2.2466 -2.2327
C -2.9461 -2.7291 -0.8046
C -3.7566 -3.5556 -0.0513
H -4.6660 -4.0403 -0.3960
C -3.1480 -3.6986 1.2296
H -3.5067 -4.3148 2.0487
C -1.9820 -2.9558 1.2215
C -0.9499 -2.7460 2.3131
C -1.1531 -1.3873 2.9520
C -1.6913 -1.0611 4.1804
H -2.0504 -1.7657 4.9251
C -1.6346 0.3572 4.3095
H -1.9429 0.9421 5.1713
C -1.0645 0.8558 3.1555
C -0.7683 2.2883 2.7622
C -1.7995 2.7617 1.7569
C -2.9115 3.5661 1.9182
H -3.2241 4.0429 2.8428

C	-3.5293	3.7040	0.6398
H	-4.4007	4.3076	0.4014
C	-2.7771	2.9786	-0.2632
C	-2.9379	2.7857	-1.7570
C	-4.1264	-3.1317	-2.9453
H	-3.8268	-4.1861	-2.8989
H	-4.2177	-2.8288	-3.9982
H	-5.1154	-3.0432	-2.4761
C	-1.1612	-3.8274	3.3786
H	-0.4839	-3.6780	4.2279
H	-0.9830	-4.8213	2.9445
H	-2.1886	-3.8011	3.7653
C	-0.8653	3.1745	4.0080
H	-1.8727	3.1335	4.4439
H	-0.6496	4.2186	3.7424
H	-0.1552	2.8441	4.7768
C	-3.8990	3.8530	-2.2900
H	-4.8955	3.7421	-1.8416
H	-4.0007	3.7591	-3.3806
H	-3.5340	4.8586	-2.0472
C	-1.7347	-2.3181	-2.9567
H	-1.8319	-1.8085	-3.9301
H	-0.9918	-1.7358	-2.3860
C	-1.2207	-3.7411	-3.1679
H	-1.7975	-4.2142	-3.9772
H	-1.4126	-4.3401	-2.2598
C	0.2693	-3.8007	-3.4997
H	0.4967	-4.7659	-3.9815
H	0.5145	-3.0222	-4.2443
C	1.1813	-3.6431	-2.2871
H	0.9273	-4.4194	-1.5429
H	1.0088	-2.6693	-1.7926
C	2.6564	-3.7543	-2.6561
H	2.8257	-4.7074	-3.1860
H	2.8996	-2.9530	-3.3733
C	3.5791	-3.6592	-1.4494
H	4.6396	-3.7434	-1.7318
H	3.3649	-4.4601	-0.7244
H	3.4364	-2.6943	-0.9388
C	0.4747	-2.8524	1.7147
H	0.5652	-3.8405	1.2321
H	0.5931	-2.1116	0.9035
C	1.6066	-2.6630	2.7221
H	1.5016	-3.3861	3.5467
H	1.5297	-1.6614	3.1823
C	2.9869	-2.8363	2.0969
H	3.0402	-3.8210	1.5995
H	3.1175	-2.0893	1.2960
C	4.1265	-2.7267	3.1059
H	4.1237	-1.7160	3.5505
H	3.9378	-3.4241	3.9391
C	5.5050	-3.0168	2.5111
H	6.2659	-2.9013	3.2991
H	5.5469	-4.0736	2.1971
C	5.8605	-2.1270	1.3232
H	6.9009	-2.2809	1.0024
H	5.7433	-1.0601	1.5744
H	5.2144	-2.3372	0.4583
C	0.6376	2.4103	2.1302
H	0.6484	1.9147	1.1442
H	0.8165	3.4796	1.9243

C	1.7944	1.8365	2.9414
H	1.6862	0.7394	3.0061
H	1.7734	2.2030	3.9807
C	3.1348	2.1868	2.2999
H	3.0595	2.0398	1.2094
H	3.3303	3.2623	2.4484
C	4.3007	1.3578	2.8244
H	4.0655	0.2907	2.6601
H	4.3890	1.4867	3.9183
C	5.6400	1.6769	2.1605
H	6.4056	0.9880	2.5521
H	5.5615	1.4645	1.0797
C	6.1099	3.1149	2.3604
H	7.1152	3.2659	1.9426
H	6.1483	3.3705	3.4309
H	5.4385	3.8334	1.8686
C	-1.5568	2.9067	-2.4465
H	-0.8624	2.1716	-2.0047
H	-1.6709	2.6147	-3.5040
C	-0.9465	4.3043	-2.3605
H	-1.0724	4.6988	-1.3363
H	-1.5104	4.9791	-3.0223
C	0.5332	4.3589	-2.7377
H	0.7008	3.7903	-3.6699
H	0.7997	5.4036	-2.9685
C	1.4920	3.8544	-1.6604
H	1.3510	2.7727	-1.4805
H	1.2640	4.3636	-0.7064
C	2.9478	4.1159	-2.0371
H	3.0750	5.1935	-2.2377
H	3.1640	3.6009	-2.9883
C	3.9430	3.6724	-0.9731
H	4.9778	3.9258	-1.2501
H	3.8882	2.5830	-0.8215
H	3.7263	4.1567	-0.0082
O	-0.3803	0.0340	-0.4873
C	0.8300	0.0479	-1.0317
C	1.0204	0.1570	-2.4292
H	0.1411	0.2317	-3.0746
C	2.2953	0.1765	-2.9861
H	2.3817	0.2631	-4.0727
C	3.4600	0.0895	-2.2043
C	3.2712	-0.0234	-0.8213
H	4.1311	-0.0983	-0.1506
C	1.9981	-0.0432	-0.2482
H	1.8947	-0.1259	0.8389
C	4.8428	0.1189	-2.8687
C	5.0046	1.4047	-3.6944
C	4.9992	-1.0911	-3.8028
H	4.9448	-2.0299	-3.2341
H	4.2112	-1.1107	-4.5706
H	5.9726	-1.0536	-4.3164
H	4.2244	1.4962	-4.4644
H	5.9815	1.4087	-4.2027
H	4.9511	2.2907	-3.0468
C	5.9687	0.0750	-1.8321
H	5.9290	-0.8432	-1.2272
H	6.9436	0.1018	-2.3412
H	5.9209	0.9393	-1.1518

Na^+**1**:**3b**; E(RM062X) = -1934.09357017 A.U.

Na	-1.8888	0.0303	0.0002
N	-0.9484	0.0107	2.6148
H	0.0558	-0.0121	2.5312
C	-1.6923	1.1586	2.5540
N	-0.8781	2.4691	-0.0001
H	-0.2318	1.6661	-0.0001
C	-3.0120	0.7699	2.4676
H	-3.8570	1.4371	2.4179
N	-0.9484	0.0105	-2.6151
H	0.0558	-0.0123	-2.5316
C	-3.0451	-0.6521	2.4675
H	-3.9199	-1.2797	2.4184
N	-0.9898	-2.4517	0.0000
H	-0.3044	-1.6817	-0.0001
C	-1.7446	-1.1016	2.5535
C	-1.1916	-2.5138	2.5005
C	-1.8913	-3.3716	3.5582
H	-2.9691	-3.3865	3.4016
H	-1.6949	-2.9674	4.5506
H	-1.5215	-4.3965	3.5157
C	0.3180	-2.5138	2.7728
H	0.6926	-3.5357	2.7295
H	0.5307	-2.1104	3.7646
H	0.8690	-1.9306	2.0328
C	-1.4748	-3.0750	1.1258
C	-2.2678	-4.1126	0.7132
H	-2.8093	-4.7877	1.3542
C	-2.2678	-4.1127	-0.7131
H	-2.8094	-4.7878	-1.3539
C	-1.4748	-3.0751	-1.1258
C	-1.1917	-2.5140	-2.5005
C	0.3178	-2.5140	-2.7729
H	0.5306	-2.1107	-3.7647
H	0.6924	-3.5360	-2.7296
H	0.8689	-1.9308	-2.0329
C	-1.8916	-3.3718	-3.5580
H	-2.9694	-3.3866	-3.4015
H	-1.5218	-4.3967	-3.5155
H	-1.6952	-2.9676	-4.5506
C	-1.7447	-1.1017	-2.5535
C	-3.0450	-0.6521	-2.4671
H	-3.9199	-1.2797	-2.4177
C	-3.0119	0.7699	-2.4672
H	-3.8568	1.4372	-2.4172
C	-1.6922	1.1584	-2.5540
C	-1.0747	2.5438	-2.5012
C	-1.7366	3.4337	-3.5568
H	-1.5581	3.0236	-4.5502
H	-1.3225	4.4414	-3.5118
H	-2.8127	3.4953	-3.3998
C	0.4325	2.4746	-2.7780
H	0.9583	1.8630	-2.0426
H	0.8550	3.4777	-2.7316
H	0.6232	2.0658	-3.7720
C	-1.3292	3.1172	-1.1259
C	-2.0675	4.1945	-0.7133
H	-2.5729	4.8967	-1.3545
C	-2.0675	4.1946	0.7130
H	-2.5730	4.8967	1.3541
C	-1.3294	3.1172	1.1256
C	-1.0748	2.5439	2.5010

C	-1.7368	3.4339	3.5564
H	-2.8129	3.4955	3.3994
H	-1.3228	4.4417	3.5114
H	-1.5584	3.0239	4.5500
C	0.4324	2.4749	2.7779
H	0.6230	2.0661	3.7720
H	0.8548	3.4779	2.7315
H	0.9582	1.8632	2.0425
O	0.4327	-0.0205	-0.0002
C	1.7562	-0.0486	-0.0001
C	2.4802	-1.2532	-0.0001
H	1.9378	-2.1923	-0.0001
C	3.8693	-1.2716	-0.0000
H	4.3613	-2.2348	-0.0000
C	4.6241	-0.1027	0.0000
C	3.9086	1.0969	0.0000
H	4.4440	2.0394	0.0001
C	2.5262	1.1334	-0.0000
H	2.0181	2.0915	-0.0000
C	6.1513	-0.0844	0.0001
C	6.6579	0.6475	1.2505
C	6.6580	0.6477	-1.2502
H	6.3187	0.1413	-2.1549
H	6.2961	1.6754	-1.2839
H	7.7498	0.6744	-1.2586
H	6.2960	1.6752	1.2843
H	7.7497	0.6743	1.2589
H	6.3186	0.1410	2.1551
C	6.7423	-1.4940	0.0000
H	6.4388	-2.0555	-0.8849
H	7.8315	-1.4317	0.0000
H	6.4388	-2.0556	0.8849

$Na(1,2\text{-}DCE)_2^+$**1**:**3b**; E(RM062X) = -3932.14735759 A.U.

N	0.1086	-0.8205	-1.9619
H	-0.7221	-0.6140	-1.3972
C	0.5769	-0.0300	-2.9876
N	-0.3687	2.2059	-0.9591
H	-1.0384	1.4736	-0.6813
C	1.5707	-0.7305	-3.6213
H	2.1480	-0.3843	-4.4616
N	-0.3540	1.1873	2.1026
H	-1.0736	0.7872	1.4916
C	1.6912	-1.9925	-2.9755
H	2.3667	-2.7887	-3.2422
N	0.0826	-1.8512	1.0844
H	-0.7124	-1.2943	0.7372
C	0.7607	-2.0342	-1.9689
C	0.3427	-3.1678	-1.0624
C	1.0674	-4.4422	-1.4951
H	2.1502	-4.3409	-1.4145
H	0.8208	-4.6723	-2.5309
H	0.7551	-5.2771	-0.8687
C	-1.1738	-3.3936	-1.2070
H	-1.4886	-4.2149	-0.5620
H	-1.4123	-3.6434	-2.2414
H	-1.7502	-2.5101	-0.9333
C	0.6777	-2.8776	0.3807
C	1.5123	-3.5385	1.2433
H	2.1249	-4.3904	0.9945
C	1.4061	-2.9078	2.5149

H	1.9284	-3.1855	3.4150
C	0.5088	-1.8800	2.3957
C	-0.0350	-0.9348	3.4396
C	-1.5637	-1.1018	3.5331
H	-1.9619	-0.4484	4.3102
H	-1.8085	-2.1361	3.7772
H	-2.0606	-0.8500	2.5957
C	0.5812	-1.2879	4.7930
H	1.6664	-1.1846	4.7721
H	0.3367	-2.3167	5.0551
H	0.1848	-0.6279	5.5634
C	0.2794	0.5093	3.1228
C	1.0627	1.4185	3.7874
H	1.6856	1.2079	4.6398
C	0.8670	2.6877	3.1764
H	1.3285	3.6157	3.4685
C	-0.0208	2.5232	2.1445
C	-0.6252	3.5256	1.1881
C	-0.2671	4.9336	1.6621
H	-0.6455	5.0915	2.6713
H	-0.7148	5.6736	0.9995
H	0.8126	5.0844	1.6689
C	-2.1567	3.3723	1.1925
H	-2.4697	2.3736	0.8865
H	-2.6029	4.0909	0.5040
H	-2.5444	3.5535	2.1955
C	-0.0992	3.3373	-0.2171
C	0.6619	4.1671	-0.9975
H	1.0465	5.1287	-0.7013
C	0.8436	3.5308	-2.2568
H	1.3795	3.9259	-3.1035
C	0.1863	2.3287	-2.2169
C	-0.0439	1.3089	-3.3089
C	0.5660	1.8335	-4.6081
H	1.6407	1.9883	-4.5053
H	0.1031	2.7816	-4.8790
H	0.3949	1.1190	-5.4123
C	-1.5588	1.1157	-3.5133
H	-1.7356	0.4227	-4.3364
H	-2.0286	2.0724	-3.7452
H	-2.0404	0.7082	-2.6235
O	-1.7968	-0.0345	-0.0021
C	-3.1167	-0.2274	-0.0520
C	-3.7159	-1.3716	0.4882
H	-3.0878	-2.1209	0.9565
C	-5.0901	-1.5655	0.4314
H	-5.4917	-2.4711	0.8652
C	-5.9405	-0.6371	-0.1611
C	-5.3411	0.5047	-0.6977
H	-5.9576	1.2615	-1.1688
C	-3.9743	0.7114	-0.6495
H	-3.5488	1.6128	-1.0759
C	-7.4552	-0.8154	-0.2419
C	-7.8973	-0.8103	-1.7118
C	-8.1489	0.3384	0.4954
H	-7.8570	0.3523	1.5465
H	-7.8865	1.3031	0.0608
H	-9.2339	0.2266	0.4394
H	-7.6312	0.1247	-2.2050
H	-8.9802	-0.9329	-1.7822
H	-7.4211	-1.6258	-2.2580

C	-7.9127	-2.1300	0.3894
H	-7.6533	-2.1768	1.4481
H	-8.9972	-2.2171	0.3060
H	-7.4675	-2.9902	-0.1127
Cs	1.3962	0.4825	0.2100
Cl	3.5281	0.8824	-1.7988
Cl	3.1198	2.7860	0.9978
C	4.1514	3.1447	-0.4118
C	4.7606	1.8947	-0.9929
H	4.9371	3.8105	-0.0619
H	3.5195	3.6545	-1.1358
H	5.4857	2.1586	-1.7593
H	5.2327	1.2865	-0.2255
Cl	3.8788	-0.5056	1.5661
H	4.8495	-1.6298	-0.9771
C	4.3079	-2.3435	-0.3636
C	4.5326	-2.1119	1.1099
Cl	4.9056	-3.9744	-0.7768
H	3.2491	-2.3087	-0.6117
H	4.0028	-2.8442	1.7090
H	5.5887	-2.1035	1.3623

$Na(1,2\text{-}DCE)_2^+$**2**:**3b**; E(RM062X) = -2720.26234680 A.U.

Na	-2.8266	0.0193	1.0978
N	-3.3537	0.2883	-1.4650
H	-2.3653	0.2063	-1.1600
C	-4.0343	1.4742	-1.6349
N	-1.8988	2.6481	0.8367
H	-1.0496	2.6307	0.2816
C	-5.2754	1.1717	-2.1488
H	-6.0597	1.8851	-2.3847
N	-0.7502	-0.2447	2.6798
H	-0.5742	-0.1651	1.6612
C	-5.3483	-0.2482	-2.2862
H	-6.1986	-0.8200	-2.6463
N	-2.1738	-2.6024	0.3440
H	-1.3149	-2.5635	-0.1959
C	-4.1493	-0.7678	-1.8520
C	-3.6929	-2.2017	-1.6713
C	-3.4245	-2.4142	-0.1870
C	-4.3065	-2.3540	0.8803
H	-5.3819	-2.2126	0.7995
C	-3.5463	-2.5021	2.0768
H	-3.9218	-2.4966	3.0976
C	-2.2166	-2.6508	1.7129
C	-0.9841	-2.7334	2.6035
C	-0.9016	-1.4291	3.3641
C	-1.0044	-1.1296	4.7026
H	-1.1410	-1.8476	5.5066
C	-0.9139	0.2937	4.8297
H	-0.9693	0.8697	5.7494
C	-0.7604	0.8099	3.5640
C	-0.6936	2.2292	3.0469
C	-1.9354	2.4486	2.1922
C	-3.2737	2.3789	2.5481
H	-3.6490	2.2256	3.5576
C	-4.0450	2.5362	1.3590
H	-5.1295	2.5291	1.2753
C	-3.1605	2.6964	0.3038
C	-3.4365	2.7945	-1.1909
C	-4.8211	-3.1401	-2.1197

H	-4.5576	-4.1863	-1.9202
H	-5.0135	-3.0182	-3.1962
H	-5.7483	-2.9165	-1.5752
C	-1.1619	-3.8981	3.5861
H	-0.3258	-3.9484	4.2963
H	-1.2192	-4.8470	3.0348
H	-2.0897	-3.7805	4.1620
C	-0.7088	3.2118	4.2238
H	-1.6286	3.0989	4.8136
H	-0.6658	4.2442	3.8502
H	0.1474	3.0374	4.8900
C	-4.4581	3.9114	-1.4419
H	-5.4083	3.6849	-0.9400
H	-4.6524	4.0166	-2.5198
H	-4.0899	4.8679	-1.0501
C	-2.4170	-2.4469	-2.5061
H	-2.5959	-2.0427	-3.5157
H	-1.5966	-1.8356	-2.0915
C	-1.9880	-3.9101	-2.6264
H	-2.7073	-4.4381	-3.2702
H	-2.0412	-4.4085	-1.6422
C	-0.5824	-4.0759	-3.2007
H	-0.4446	-5.1222	-3.5192
H	-0.4859	-3.4629	-4.1139
C	0.5451	-3.7172	-2.2356
H	0.4284	-4.3058	-1.3063
H	0.4941	-2.6502	-1.9460
C	1.9216	-3.9915	-2.8347
H	1.9722	-5.0467	-3.1527
H	2.0308	-3.3894	-3.7523
C	3.0627	-3.6809	-1.8771
H	4.0459	-3.8611	-2.3372
H	3.0002	-4.3012	-0.9703
H	3.0192	-2.6253	-1.5644
C	0.2999	-2.9250	1.7620
H	0.2675	-3.9219	1.2878
H	0.3216	-2.1844	0.9416
C	1.5906	-2.7668	2.5613
H	1.5816	-3.4335	3.4392
H	1.6379	-1.7404	2.9657
C	2.8442	-3.0400	1.7393
H	2.8197	-4.0781	1.3623
H	2.8363	-2.3911	0.8464
C	4.1265	-2.8265	2.5387
H	4.1464	-1.7884	2.9149
H	4.1006	-3.4708	3.4334
C	5.4095	-3.1005	1.7554
H	6.2711	-2.9909	2.4327
H	5.4141	-4.1523	1.4220
C	5.5918	-2.1849	0.5487
H	6.5636	-2.3473	0.0607
H	5.5405	-1.1239	0.8451
H	4.8108	-2.3574	-0.2061
C	0.5836	2.4217	2.1995
H	0.4804	1.8732	1.2466
H	0.6782	3.4910	1.9394
C	1.8727	1.9248	2.8464
H	1.8026	0.8313	2.9829
H	1.9972	2.3447	3.8580
C	3.0914	2.2563	1.9895
H	2.8481	2.0598	0.9317

H	3.2989	3.3376	2.0601
C	4.3319	1.4504	2.3596
H	4.0831	0.3778	2.2705
H	4.5836	1.6182	3.4221
C	5.5526	1.7498	1.4899
H	6.3588	1.0457	1.7513
H	5.2975	1.5450	0.4349
C	6.0753	3.1776	1.6203
H	6.9983	3.3181	1.0405
H	6.2987	3.4179	2.6713
H	5.3444	3.9139	1.2565
C	-2.1339	3.0597	-1.9786
H	-1.3854	2.2961	-1.7023
H	-2.3477	2.8800	-3.0447
C	-1.5506	4.4650	-1.8207
H	-1.5410	4.7621	-0.7569
H	-2.2155	5.1812	-2.3261
C	-0.1418	4.6018	-2.3953
H	-0.1186	4.1752	-3.4136
H	0.0937	5.6727	-2.5088
C	0.9640	3.9593	-1.5593
H	0.8223	2.8637	-1.4866
H	0.9169	4.3559	-0.5276
C	2.3456	4.2431	-2.1440
H	2.4655	5.3338	-2.2590
H	2.3880	3.8232	-3.1629
C	3.4894	3.6873	-1.3074
H	4.4695	3.9134	-1.7541
H	3.4021	2.5934	-1.2112
H	3.4757	4.1143	-0.2932
O	-0.8851	0.0186	-0.1389
C	0.2108	0.0439	-0.8680
C	0.1716	0.1799	-2.2805
H	-0.7999	0.2631	-2.7751
C	1.3337	0.2112	-3.0433
H	1.2336	0.3162	-4.1272
C	2.6137	0.1133	-2.4731
C	2.6587	-0.0230	-1.0792
H	3.6196	-0.1101	-0.5649
C	1.5015	-0.0605	-0.2982
H	1.5915	-0.1676	0.7887
C	3.8615	0.1400	-3.3654
C	3.8994	1.4388	-4.1864
C	3.8312	-1.0536	-4.3338
H	3.8422	-2.0016	-3.7789
H	2.9304	-1.0370	-4.9653
H	4.7103	-1.0309	-4.9968
H	2.9963	1.5555	-4.8033
H	4.7703	1.4367	-4.8602
H	3.9786	2.3131	-3.5262
C	5.1479	0.0582	-2.5393
H	5.1983	-0.8757	-1.9599
H	6.0220	0.0890	-3.2064
H	5.2291	0.9035	-1.8384

$Cs(1,2\text{-}DCE)_2^+$**2**:**3b (less stable complex, Figure S5b)**; E(RM062X) = -2578.11570839 A.U.

Cs	-4.0741	-0.0001	-0.1426
N	-1.9576	-0.0002	2.3369
H	-1.1559	-0.0001	1.6841
C	-2.6049	1.1270	2.7834
N	-1.8177	2.3874	-0.0352

H	-1.0682	1.6777	0.0019
C	-3.7041	0.7128	3.5107
H	-4.4059	1.3595	4.0296
N	-1.7096	-0.0001	-2.4035
H	-0.9981	-0.0001	-1.6521
C	-2.0914	2.5188	2.4740
C	-2.4771	2.8943	1.0595
C	-3.4763	3.7260	0.5950
H	-4.1595	4.3044	1.2107
C	-3.4040	3.7262	-0.8295
H	-4.0215	4.3053	-1.5104
C	-2.3629	2.8943	-1.1906
C	-1.8301	2.5240	-2.5579
C	-2.2991	1.1280	-2.9239
C	-3.3019	0.7129	-3.7788
H	-3.9368	1.3585	-4.3789
C	-2.7330	3.5103	3.4474
H	-2.4275	4.5371	3.2085
H	-2.4329	3.2739	4.4782
H	-3.8292	3.4654	3.3902
C	-2.3784	3.5113	-3.5911
H	-3.4750	3.4634	-3.6377
H	-1.9821	3.2725	-4.5880
H	-2.1005	4.5400	-3.3286
C	-0.5538	2.5211	2.6283
H	-0.3130	2.1149	3.6254
H	-0.1173	1.8146	1.9026
C	0.1360	3.8675	2.4443
H	-0.1419	4.5537	3.2611
H	-0.2071	4.3405	1.5071
C	1.6524	3.7002	2.4164
H	1.9684	3.1386	3.3154
H	1.9225	3.0611	1.5573
C	2.4221	5.0153	2.3553
H	2.0407	5.6973	3.1337
H	2.2178	5.5114	1.3900
C	-0.2839	2.5368	-2.5534
H	0.0765	1.7867	-1.8321
H	0.0566	2.1896	-3.5442
C	0.3917	3.8600	-2.2120
H	0.0694	4.6531	-2.9064
H	0.0840	4.1837	-1.2022
C	1.9126	3.7303	-2.2726
H	2.2366	2.9041	-1.6144
H	2.2053	3.4324	-3.2954
C	2.6588	5.0026	-1.8886
H	2.4691	5.2260	-0.8235
H	2.2531	5.8603	-2.4538
C	4.1635	4.9110	-2.1265
H	4.5498	3.9945	-1.6489
H	4.3492	4.7850	-3.2062
C	4.9224	6.1267	-1.6082
H	6.0012	6.0479	-1.8027
H	4.7842	6.2416	-0.5215
H	4.5597	7.0498	-2.0854
C	3.9311	4.8450	2.5317
H	4.4183	5.8282	2.4310
H	4.1368	4.5054	3.5610
C	4.5507	3.8629	1.5423
H	5.6481	3.8545	1.6171
H	4.2862	4.1304	0.5068

H	4.1950	2.8343	1.7086
C	-2.6047	-1.1276	2.7833
N	-1.8174	-2.3876	-0.0354
H	-1.0682	-1.6777	0.0018
C	-3.7039	-0.7137	3.5106
H	-4.4057	-1.3605	4.0296
C	-2.0910	-2.5193	2.4739
C	-2.4767	-2.8948	1.0593
C	-3.4755	-3.7270	0.5949
H	-4.1585	-4.3056	1.2106
C	-3.4032	-3.7270	-0.8297
H	-4.0206	-4.3063	-1.5105
C	-2.3625	-2.8947	-1.1908
C	-1.8298	-2.5242	-2.5580
C	-2.2989	-1.1283	-2.9239
C	-3.3018	-0.7133	-3.7788
H	-3.9366	-1.3590	-4.3790
C	-2.7324	-3.5109	3.4473
H	-2.4268	-4.5377	3.2082
H	-2.4322	-3.2746	4.4780
H	-3.8286	-3.4661	3.3902
C	-2.3779	-3.5117	-3.5912
H	-3.4745	-3.4641	-3.6378
H	-1.9817	-3.2727	-4.5881
H	-2.0996	-4.5403	-3.3288
C	-0.5534	-2.5213	2.6281
H	-0.3126	-2.1150	3.6253
H	-0.1171	-1.8148	1.9024
C	0.1368	-3.8676	2.4442
H	-0.1410	-4.5538	3.2610
H	-0.2062	-4.3407	1.5071
C	1.6531	-3.6999	2.4163
H	1.9690	-3.1382	3.3153
H	1.9231	-3.0608	1.5572
C	2.4231	-5.0148	2.3552
H	2.0419	-5.6968	3.1337
H	2.2188	-5.5110	1.3900
C	-0.2836	-2.5369	-2.5535
H	0.0767	-1.7867	-1.8323
H	0.0569	-2.1897	-3.5443
C	0.3923	-3.8599	-2.2118
H	0.0701	-4.6531	-2.9062
H	0.0845	-4.1836	-1.2020
C	1.9131	-3.7299	-2.2725
H	2.2369	-2.9035	-1.6145
H	2.2058	-3.4322	-3.2953
C	2.6596	-5.0020	-1.8881
H	2.4702	-5.2250	-0.8230
H	2.2541	-5.8600	-2.4530
C	4.1643	-4.9101	-2.1264
H	4.5506	-3.9935	-1.6489
H	4.3497	-4.7841	-3.2061
C	4.9235	-6.1256	-1.6083
H	6.0023	-6.0465	-1.8027
H	4.7853	-6.2408	-0.5216
H	4.5610	-7.0487	-2.0855
C	3.9321	-4.8443	2.5315
H	4.4194	-5.8273	2.4308
H	4.1378	-4.5045	3.5607
C	4.5513	-3.8621	1.5419
H	5.6487	-3.8532	1.6167

H 4.2870 -4.1299 0.5064
H 4.1953 -2.8336 1.7079
O -0.2138 -0.0000 0.0471
C 5.5255 0.0003 0.0207
C 1.1156 0.0000 0.0609
C 1.8686 0.0001 -1.1366
H 1.3395 0.0000 -2.0926
C 3.2579 0.0002 -1.1231
H 3.7826 0.0002 -2.0822
C 3.9942 0.0002 0.0709
C 3.2537 0.0001 1.2594
H 3.7663 0.0002 2.2229
C 1.8568 0.0001 1.2610
H 1.3169 0.0000 2.2120
C 6.1413 0.0003 1.4223
C 6.0150 -1.2522 -0.7247
H 5.6282 -1.2852 -1.7538
H 5.6826 -2.1644 -0.2084
H 7.1151 -1.2636 -0.7765
H 7.2387 0.0003 1.3447
H 5.8438 0.8930 1.9929
H 5.8438 -0.8924 1.9929
C 6.0148 1.2530 -0.7246
H 5.6279 1.2861 -1.7536
H 5.6824 2.1650 -0.2081
H 7.1149 1.2646 -0.7765

Cs^+:**3b**; E(RM062X) = -484.233495827 A.U.

Cs -3.7951 -0.0033 0.0003
O -1.2969 -0.0014 -0.0001
C 4.4067 -0.0006 -0.0002
C 0.0085 0.0124 -0.0004
C 0.7680 -1.1784 -0.0001
H 0.2335 -2.1211 0.0000
C 2.1496 -1.1578 -0.0001
H 2.6770 -2.1059 0.0000
C 2.8796 0.0348 -0.0003
C 2.1364 1.2131 -0.0003
H 2.6411 2.1706 -0.0004
C 0.7485 1.2094 -0.0004
H 0.2016 2.1450 -0.0004
C 5.0151 1.4019 -0.0002
C 4.9097 -0.7369 1.2494
H 4.5325 -1.7590 1.2851
H 4.5768 -0.2248 2.1534
H 6.0017 -0.7782 1.2569
H 6.1041 1.3280 -0.0001
H 4.7160 1.9664 -0.8847
H 4.7158 1.9665 0.8842
C 4.9099 -0.7370 -1.2496
H 4.5327 -1.7592 -1.2853
H 4.5770 -0.2250 -2.1537
H 6.0019 -0.7783 -1.2570

$Cs(1,2\text{-}DCE)_2^+$:**3b**; E(RM062X) = -2482.30385121 A.U.

O -0.3552 0.6090 -0.9773
C 5.2609 0.6039 -0.0079
C 0.9294 0.6824 -0.7874
C 1.8576 0.0923 -1.6781
H 1.4694 -0.3796 -2.5722

C	3.2111	0.0789	-1.4093
H	3.8702	-0.4041	-2.1224
C	3.7553	0.6588	-0.2551
C	2.8545	1.2784	0.6074
H	3.2112	1.7580	1.5098
C	1.4881	1.2983	0.3527
H	0.8118	1.7690	1.0602
C	5.6526	1.2886	1.3010
C	5.7215	-0.8590	0.0620
H	5.4930	-1.3935	-0.8603
H	5.2233	-1.3776	0.8834
H	6.8003	-0.9135	0.2252
H	6.7327	1.2220	1.4416
H	5.3800	2.3451	1.2958
H	5.1721	0.8141	2.1582
C	6.0006	1.3062	-1.1552
H	5.7899	0.8312	-2.1134
H	5.6945	2.3509	-1.2239
H	7.0801	1.2717	-0.9910
Cs	-2.5396	-0.9036	-0.9336
Cl	-2.3733	1.2228	1.9918
Cl	-3.6462	2.4730	-0.8719
C	-2.0992	2.9700	-0.1038
C	-2.1906	2.9019	1.3967
H	-1.9256	3.9983	-0.4119
H	-1.3272	2.3019	-0.4932
H	-1.2659	3.2805	1.8270
H	-3.0351	3.4626	1.7865
Cl	-1.3343	-2.2082	2.1983
Cl	0.4035	-2.8780	-0.5635
C	1.0959	-2.1374	0.9122
C	0.0998	-1.2758	1.6430
H	1.9299	-1.5151	0.5859
H	1.4463	-2.9605	1.5279
H	0.5630	-0.8604	2.5347
H	-0.2650	-0.4638	1.0206

$Cs(1,2\text{-}DCE)_3^+$:**3b**; E(RM062X) = -3481.33328936 A.U.

O	-0.1360	0.4455	0.6222
C	5.5660	0.5166	0.7916
C	1.1621	0.5066	0.7192
C	1.9404	1.3815	-0.0781
H	1.4285	2.0300	-0.7798
C	3.3220	1.3712	-0.0315
H	3.8604	2.0504	-0.6839
C	4.0391	0.5062	0.8032
C	3.2811	-0.3392	1.6119
H	3.7727	-1.0280	2.2867
C	1.8930	-0.3376	1.5816
H	1.3358	-1.0266	2.2076
C	6.1552	-0.4915	1.7779
C	6.0723	0.1619	-0.6139
H	5.7011	0.8664	-1.3586
H	5.7383	-0.8374	-0.8995
H	7.1640	0.1804	-0.6448
H	7.2448	-0.4509	1.7357
H	5.8505	-0.2726	2.8024
H	5.8488	-1.5111	1.5385
C	6.0795	1.9126	1.1700
H	5.7180	2.6700	0.4744
H	5.7414	2.1859	2.1705

H 7.1715 1.9344 1.1560
Cs -2.0917 -0.3877 -1.1040
Cl -0.1328 -3.4086 -1.6447
Cl 1.0332 -0.4995 -2.8030
C 1.9495 -1.6140 -1.7437
C 1.0513 -2.3593 -0.7936
H 2.6381 -0.9973 -1.1654
H 2.4925 -2.2861 -2.4016
H 1.6488 -3.0108 -0.1602
H 0.4845 -1.6812 -0.1642
Cl -4.0390 -0.6897 1.8989
Cl -1.4427 -2.7306 1.6017
C -1.7529 -1.6846 3.0162
C -2.4321 -0.3944 2.6380
H -0.7842 -1.4545 3.4542
H -2.3478 -2.2708 3.7105
H -2.6130 0.1979 3.5321
H -1.8200 0.1725 1.9373
Cl -3.3721 2.4843 0.7718
Cl -1.2096 3.0005 -1.7895
C -0.9370 3.3905 -0.0611
C -2.2097 3.8347 0.6069
H -0.2063 4.1958 -0.0402
H -0.5359 2.4840 0.3942
H -1.9885 4.1717 1.6170
H -2.7150 4.6235 0.0574

$Cs(1,2\text{-}DCE)_3^+$; E(RM062X) = -3017.03400806 A.U.

Cs 0.0139 -0.5010 -1.5836
Cl -1.8778 -2.2711 0.7919
C -3.1859 -1.2897 1.5172
Cl 0.0107 0.5206 1.7934
C 0.3265 2.2775 1.9351
Cl 2.2153 -2.2113 0.5329
Cl -3.0914 0.6630 -0.3961
C -4.0209 -0.5974 0.4730
Cl -0.2325 2.8585 -0.6814
C -0.5936 3.0837 1.0569
Cl 2.9616 0.9909 -0.3066
C 3.3437 -1.1208 1.3910
C 4.0684 -0.2004 0.4454
H 4.0600 -1.7637 1.8968
H 2.7570 -0.5723 2.1218
H 4.8106 0.3773 0.9911
H 4.5496 -0.7436 -0.3621
H 1.3711 2.4318 1.6780
H 0.1562 2.5359 2.9775
H -1.6348 2.8100 1.2018
H -0.4565 4.1437 1.2558
H -2.7121 -0.5819 2.1913
H -3.8054 -1.9820 2.0821
H -4.3964 -1.2906 -0.2737
H -4.8539 -0.0862 0.9494

Na^+:**3b**; E(RM062X) = -626.392668367 A.U.

Na -5.1312 -0.0129 -0.0003
O -3.1738 -0.0057 0.0000
C 2.5260 0.0008 0.0000
C -1.8685 0.0094 0.0001
C -1.1112 -1.1806 0.0001

H	-1.6453	-2.1234	0.0001
C	0.2706	-1.1587	0.0001
H	0.7987	-2.1062	0.0001
C	0.9988	0.0347	0.0001
C	0.2550	1.2123	0.0000
H	0.7586	2.1702	-0.0000
C	-1.1330	1.2071	0.0000
H	-1.6815	2.1417	-0.0000
C	3.1329	1.4039	-0.0001
C	3.0292	-0.7351	1.2497
H	2.6536	-1.7578	1.2852
H	2.6955	-0.2236	2.1538
H	4.1211	-0.7749	1.2573
H	4.2219	1.3309	-0.0001
H	2.8336	1.9682	-0.8847
H	2.8336	1.9683	0.8844
C	3.0291	-0.7353	-1.2496
H	2.6535	-1.7580	-1.2849
H	2.6954	-0.2240	-2.1537
H	4.1211	-0.7752	-1.2572

$Na(1,2\text{-}DCE)_2^+$:**3b**; E(RM062X) = -2624.46746559 A.U.

O	-0.8990	-0.4072	-0.9527
C	4.7163	-0.7475	-0.0236
C	0.3860	-0.5574	-0.7794
C	0.9306	-1.0734	0.4196
H	0.2449	-1.3958	1.1951
C	2.2952	-1.1250	0.6326
H	2.6521	-1.5125	1.5806
C	3.2201	-0.6875	-0.3229
C	2.6921	-0.2183	-1.5238
H	3.3533	0.1150	-2.3129
C	1.3233	-0.1601	-1.7543
H	0.9449	0.2070	-2.7015
C	5.5572	-0.2457	-1.1972
C	5.0326	0.1258	1.1989
H	4.4787	-0.2056	2.0776
H	4.7648	1.1660	1.0040
H	6.0985	0.0840	1.4346
H	6.6163	-0.3062	-0.9415
H	5.3927	-0.8474	-2.0922
H	5.3291	0.7944	-1.4362
C	5.1300	-2.1951	0.2761
H	4.5899	-2.5934	1.1352
H	4.9197	-2.8378	-0.5799
H	6.1988	-2.2484	0.4949
Na	-2.3791	0.6937	0.0644
Cl	-1.5911	3.5412	-0.4956
Cl	-0.4437	1.6246	1.8774
C	0.6334	2.4020	0.6743
C	-0.0403	2.6440	-0.6552
H	1.4685	1.7163	0.5206
H	0.9682	3.3273	1.1329
H	0.6097	3.2519	-1.2796
H	-0.2742	1.7147	-1.1631
Cl	-4.4770	-0.7937	-1.2034
Cl	-2.9787	-1.5814	1.6858
C	-2.8148	-2.5072	0.1552
C	-4.0877	-2.4547	-0.6472
H	-2.6057	-3.5357	0.4395
H	-1.9725	-2.0600	-0.3777

H -3.9734 -3.0541 -1.5470
H -4.9487 -2.7939 -0.0792

$Na(1,2\text{-}DCE)_3^+$:**3b**; E(RM062X) = -3623.49543625 A.U.

O 0.4381 -0.1504 -0.8727
C -5.2546 0.0246 -0.5398
C -0.8685 -0.1062 -0.8721
C -1.5854 1.1009 -0.7057
H -1.0305 2.0264 -0.6119
C -2.9640 1.1150 -0.6109
H -3.4545 2.0711 -0.4648
C -3.7361 -0.0511 -0.6823
C -3.0395 -1.2395 -0.8855
H -3.5759 -2.1759 -0.9669
C -1.6535 -1.2706 -0.9866
H -1.1421 -2.2169 -1.1335
C -5.9108 -1.3515 -0.6462
C -5.6131 0.6197 0.8294
H -5.1923 1.6179 0.9516
H -5.2257 -0.0101 1.6325
H -6.6969 0.6935 0.9436
H -6.9913 -1.2517 -0.5317
H -5.7174 -1.8126 -1.6159
H -5.5521 -2.0260 0.1330
C -5.8366 0.9200 -1.6423
H -5.4278 1.9291 -1.5917
H -5.6054 0.5127 -2.6275
H -6.9222 0.9899 -1.5431
Na 1.9804 -0.3134 0.5793
Cl 1.0404 -1.9267 2.9889
Cl 0.1059 1.1300 2.2343
C -1.0466 -0.2222 2.4357
C -0.4485 -1.5532 2.0556
H -1.8889 -0.0171 1.7733
H -1.3599 -0.2063 3.4755
H -1.1604 -2.3472 2.2668
H -0.1849 -1.5870 1.0029
Cl 3.6311 -0.8480 -1.7494
Cl 2.0404 -3.2240 -0.0435
C 2.3760 -3.2661 -1.8010
C 2.3349 -1.8944 -2.4217
H 1.6027 -3.8861 -2.2488
H 3.3451 -3.7422 -1.9193
H 2.5233 -1.9700 -3.4899
H 1.4024 -1.3712 -2.2075
Cl 3.5679 1.9812 0.6160
Cl 0.9595 3.9670 -0.0746
C 1.7152 2.8323 -1.2221
C 3.1974 2.7142 -0.9830
H 1.5553 3.2346 -2.2209
H 1.2096 1.8679 -1.1321
H 3.6426 2.0607 -1.7288
H 3.6921 3.6809 -0.9830

$Na(1,2\text{-}DCE)_3^+$; E(RM062X) = -3159.19322180 A.U.

Na 0.0631 -0.3613 0.2413
Cl -1.2978 1.8196 1.2884
C -1.1517 3.0447 -0.0132
H -1.5695 3.9633 0.3913
H -1.7551 2.6972 -0.8472

C	0.2840	3.2688	-0.4090
H	0.3450	4.0819	-1.1280
H	0.9137	3.4839	0.4491
Cl	0.9800	1.8310	-1.2247
Cl	2.4217	-0.1237	1.6793
C	3.6419	-0.3769	0.3900
H	4.6084	-0.3689	0.8878
H	3.5678	0.4680	-0.2888
C	3.4467	-1.6907	-0.3191
H	4.2506	-1.8443	-1.0346
H	3.4025	-2.5264	0.3725
Cl	1.9278	-1.7209	-1.2738
Cl	-1.9191	-1.8670	1.4266
C	-3.3691	-1.3036	0.5347
H	-3.5158	-0.2588	0.7933
H	-4.1987	-1.8988	0.9084
C	-3.2271	-1.5062	-0.9507
H	-2.9586	-2.5283	-1.1994
H	-4.1542	-1.2357	-1.4498
Cl	-1.9585	-0.4494	-1.6550

Ligand **1** (1,3-alternate form); E(RM062X) = -1307.63248036 A.U.

N	1.7408	-1.6761	-0.1393
H	1.4834	-1.3802	-1.0687
C	1.1057	-2.6633	0.5671
N	1.6761	1.7407	0.1392
H	1.3802	1.4834	1.0685
C	1.6328	-2.6558	1.8334
H	1.3561	-3.3203	2.6343
C	2.6186	-1.6275	1.8835
H	3.2309	-1.3650	2.7295
C	2.6642	-1.0379	0.6461
C	3.5319	0.0589	0.0824
C	2.6633	1.1056	-0.5672
C	2.6558	1.6326	-1.8335
H	3.3203	1.3559	-2.6345
C	1.6275	2.6184	-1.8837
H	1.3649	3.2306	-2.7298
C	1.0379	2.6641	-0.6464
C	-0.0589	3.5319	-0.0827
C	4.4919	-0.5283	-0.9605
H	5.1146	-1.2910	-0.4944
H	5.1367	0.2527	-1.3654
C	-0.6922	4.3566	-1.2102
H	0.0531	5.0078	-1.6684
H	-1.4942	4.9734	-0.8062
C	4.3567	0.6922	1.2099
H	3.7150	1.1090	1.9863
H	5.0080	-0.0530	1.6680
C	0.5284	4.4919	0.9602
H	-0.2525	5.1367	1.3650
H	0.9873	3.9476	1.7857
N	-1.7408	1.6761	-0.1393
H	-1.4835	1.3801	-1.0686
C	-1.1056	2.6633	0.5670
N	-1.6761	-1.7407	0.1394
H	-1.3801	-1.4833	1.0687
C	-1.6326	2.6559	1.8334
H	-1.3558	3.3203	2.6342
C	-2.6186	1.6278	1.8835
H	-3.2308	1.3653	2.7296

C	-2.6641	1.0380	0.6463
C	-3.5319	-0.0589	0.0827
C	-2.6633	-1.1057	-0.5669
C	-2.6559	-1.6328	-1.8332
H	-3.3205	-1.3561	-2.6341
C	-1.6277	-2.6186	-1.8834
H	-1.3653	-3.2309	-2.7294
C	-1.0380	-2.6641	-0.6461
C	0.0589	-3.5319	-0.0825
C	-4.4920	0.5282	-0.9602
H	-5.1146	1.2910	-0.4941
H	-5.1368	-0.2527	-1.3649
C	0.6921	-4.3567	-1.2100
H	-0.0532	-5.0079	-1.6680
H	1.4941	-4.9734	-0.8061
C	-4.3566	-0.6921	1.2104
H	-3.7148	-1.1088	1.9867
H	-5.0078	0.0531	1.6684
C	-0.5282	-4.4918	0.9606
H	0.2527	-5.1366	1.3654
H	-0.9871	-3.9475	1.7861
H	-1.1090	3.7150	-1.9865
H	-3.9478	0.9871	-1.7857
H	1.1088	-3.7151	-1.9864
H	3.9477	-0.9873	-1.7860
H	1.2911	5.1145	0.4941
H	4.9734	1.4943	0.8059
H	-4.9733	-1.4943	0.8065
H	-1.2910	-5.1145	0.4946

Ligand **2** (1,3-alternate form); E(RM062X) = -2093.78856105 A.U.

N	-0.0468	-2.4256	0.8704
H	0.0257	-1.9834	1.7818
C	1.0262	-2.6977	0.0622
N	-2.3871	0.0331	0.6201
H	-2.0754	-0.0415	-0.3423
C	0.5259	-3.1382	-1.1456
H	1.1148	-3.4450	-2.0054
C	-0.8987	-3.1231	-1.0497
H	-1.6030	-3.4157	-1.8231
C	-1.2245	-2.6739	0.2139
C	-2.5539	-2.4432	0.8983
C	-2.5765	-1.0381	1.4539
C	-2.8540	-0.5356	2.7073
H	-3.0759	-1.1244	3.5931
C	-2.8381	0.8908	2.6093
H	-3.0412	1.6000	3.4069
C	-2.5484	1.2122	1.2996
C	-2.4409	2.5339	0.5774
C	-2.7357	-3.4553	2.0385
H	-2.7446	-4.4762	1.6315
H	-3.6778	-3.2790	2.5763
C	-2.7592	3.6791	1.5511
H	-3.7657	3.5704	1.9790
H	-2.6952	4.6408	1.0236
C	-3.6867	-2.5930	-0.1434
H	-3.4844	-1.8955	-0.9739
H	-3.6329	-3.6062	-0.5756
C	-3.4143	2.5567	-0.6225
H	-3.3493	3.5504	-1.0970
H	-3.0545	1.8407	-1.3811

N	0.0468	2.4255	0.8705
H	-0.0257	1.9832	1.7819
C	-1.0262	2.6976	0.0623
N	2.3871	-0.0332	0.6202
H	2.0755	0.0414	-0.3423
C	-0.5259	3.1381	-1.1455
H	-1.1148	3.4450	-2.0052
C	0.8987	3.1230	-1.0495
H	1.6031	3.4157	-1.8230
C	1.2245	2.6738	0.2141
C	2.5540	2.4431	0.8985
C	2.5765	1.0380	1.4539
C	2.8540	0.5354	2.7074
H	3.0758	1.1242	3.5931
C	2.8380	-0.8910	2.6092
H	3.0412	-1.6003	3.4069
C	2.5484	-1.2123	1.2996
C	2.4409	-2.5340	0.5772
C	2.7358	3.4551	2.0387
H	2.7447	4.4760	1.6317
H	3.6778	3.2788	2.5765
C	2.7593	-3.6792	1.5509
H	3.7658	-3.5705	1.9788
H	2.6952	-4.6409	1.0233
C	3.6867	2.5930	-0.1433
H	3.4843	1.8954	-0.9738
H	3.6329	3.6061	-0.5754
C	3.4143	-2.5567	-0.6226
H	3.3493	-3.5504	-1.0972
H	3.0545	-1.8406	-1.3812
H	-2.0367	3.6966	2.3794
H	1.9120	3.3813	2.7630
H	2.0367	-3.6968	2.3792
H	-1.9120	-3.3815	2.7628
C	-4.8707	2.2396	-0.2979
H	-4.9349	1.2538	0.1947
H	-5.2685	2.9719	0.4241
C	-5.0917	-2.3319	0.3914
H	-5.4066	-3.1619	1.0456
H	-5.0850	-1.4265	1.0226
C	-5.7481	2.2421	-1.5469
H	-5.6442	3.2125	-2.0634
H	-5.3745	1.4823	-2.2564
C	-6.1215	-2.1579	-0.7212
H	-5.8502	-1.2769	-1.3314
H	-6.0815	-3.0248	-1.4041
C	-7.2248	1.9863	-1.2646
H	-7.3413	1.0138	-0.7518
H	-7.5975	2.7479	-0.5574
C	-7.5445	-1.9901	-0.2009
H	-7.8200	-2.8748	0.3997
H	-7.5795	-1.1317	0.4939
C	-8.0875	2.0031	-2.5238
H	-7.9045	2.9437	-3.0698
H	-7.7571	1.1940	-3.1979
C	-8.5787	-1.7888	-1.3039
H	-8.3138	-0.8891	-1.8867
H	-8.5235	-2.6335	-2.0107
C	-9.5770	1.8614	-2.2336
H	-9.7894	0.9213	-1.7033
H	-9.9325	2.6866	-1.5984

H -10.1730 1.8671 -3.1569
C -9.9990 -1.6578 -0.7664
H -10.2983 -2.5658 -0.2214
H -10.0774 -0.8126 -0.0651
H -10.7274 -1.4936 -1.5730
C 5.0917 2.3318 0.3915
H 5.4066 3.1617 1.0457
H 5.0850 1.4264 1.0227
C 4.8707 -2.2395 -0.2980
H 4.9349 -1.2538 0.1947
H 5.2686 -2.9719 0.4239
C 5.7481 -2.2418 -1.5470
H 5.6443 -3.2122 -2.0636
H 5.3744 -1.4820 -2.2565
C 6.1215 2.1578 -0.7211
H 5.8502 1.2768 -1.3313
H 6.0815 3.0247 -1.4040
C 7.2248 -1.9858 -1.2647
H 7.3411 -1.0134 -0.7518
H 7.5976 -2.7475 -0.5576
C 7.5445 1.9899 -0.2009
H 7.8200 2.8745 0.3999
H 7.5795 1.1315 0.4940
C 8.0874 -2.0025 -2.5239
H 7.9046 -2.9431 -3.0700
H 7.7570 -1.1933 -3.1979
C 8.5787 1.7887 -1.3038
H 8.3138 0.8891 -1.8867
H 8.5235 2.6334 -2.0106
C 9.5770 -1.8606 -2.2337
H 9.7892 -0.9206 -1.7033
H 9.9326 -2.6859 -1.5985
H 10.1729 -1.8662 -3.1570
C 9.9990 1.6576 -0.7663
H 10.2983 2.5655 -0.2212
H 10.0774 0.8123 -0.0651
H 10.7274 1.4935 -1.5730