Supporting Information

For

Capture and Metathesis-based Release of Potassium Salts by a Multitopic Ion Receptor

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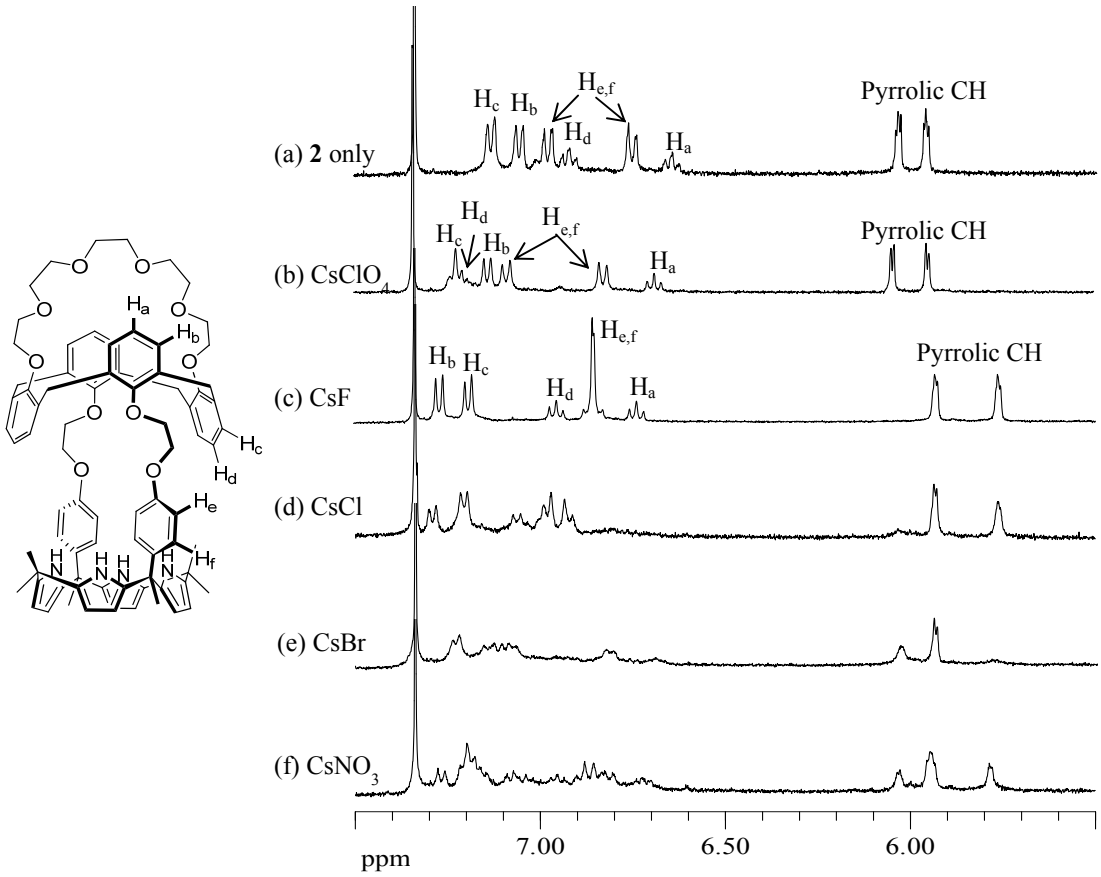

Figure S1. Partial ^{1}H NMR spectra of (a) **2** only, (b) **2** with 5.0 equiv of $CsClO_4$, (c) **2** with 5.0 equiv of CsF, (d) **2** with 5.0 equiv of CsCl, (e) **2** with 5.0 equiv of CsBr, and (f) **2** with 5.0 equiv of $CsNO_3$ in $CD_3OD/CDCl_3$ (1:9, v/v).

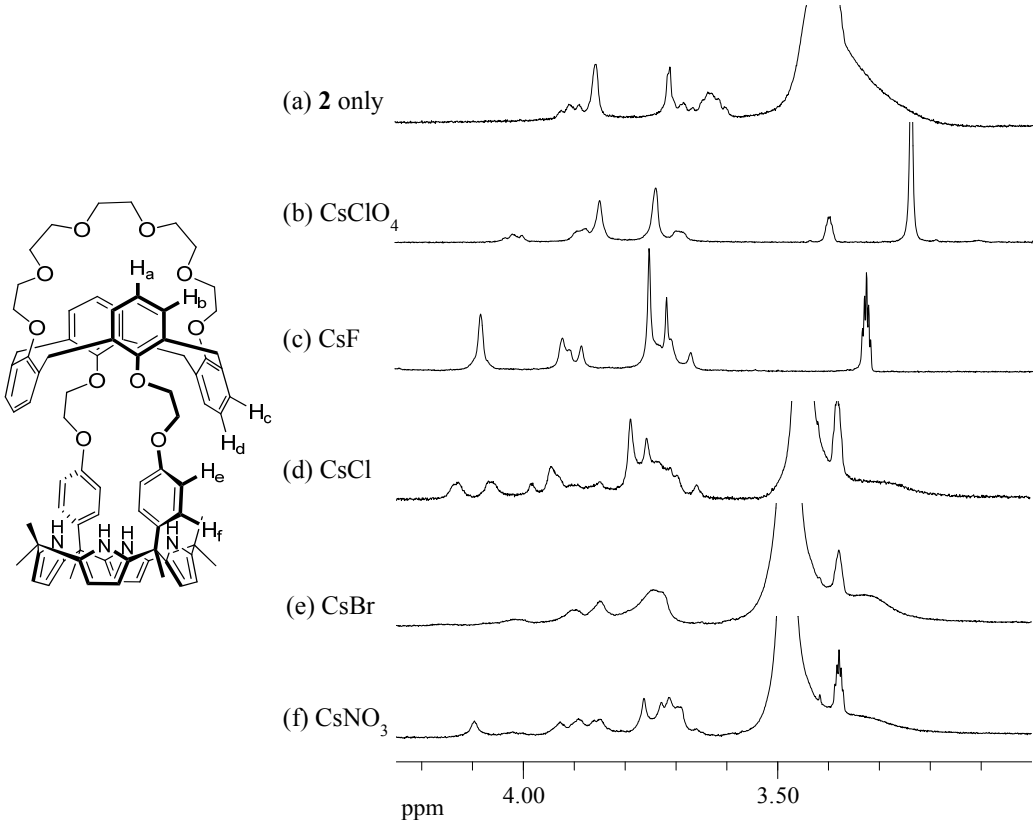

Figure S2. Partial ^{1}H NMR spectra of (a) **2** only, (b) **2** with 5.0 equiv of $CsClO_4$, (c) **2** with 5.0 equiv of CsF, (d) **2** with 5.0 equiv of CsCl, (e) **2** with 5.0 equiv of CsBr, and (f) **2** with 5.0 equiv of $CsNO_3$ in $CD_3OD/CDCl_3$ (1:9, v/v).

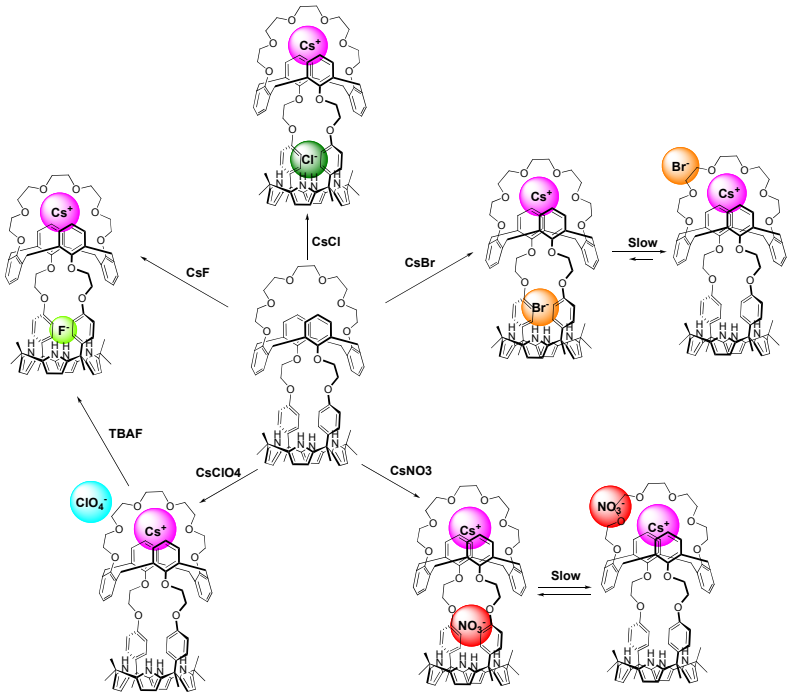

Figure S3. Proposed binding interactions involving receptor **2** and various Cs^+ ion pairs in 10% methanol in chloroform (10% CD_3OD in $CDCl_3$ for ^1H NMR spectral studies).

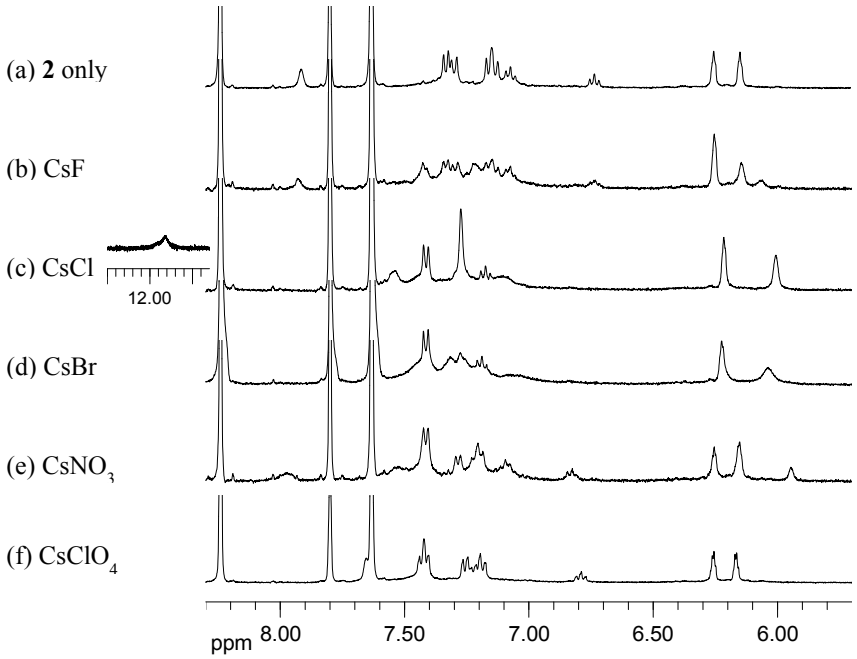

Figure S4. Partial ^{1}H NMR spectra of nitrobenzene-d_5 solutions of **2** after contacting with (a) an ion-free aqueous D_2O solution, (b) an aqueous D_2O solution of CsF (5 equiv), (c) an aqueous D_2O solution of CsCl (5 equiv), (d) an aqueous D_2O solution of CsBr (5 equiv), (e) an aqueous D_2O solution of $CsNO_3$ (5 equiv), and (f) an aqueous D_2O solution of $CsClO_4$ (5 equiv).

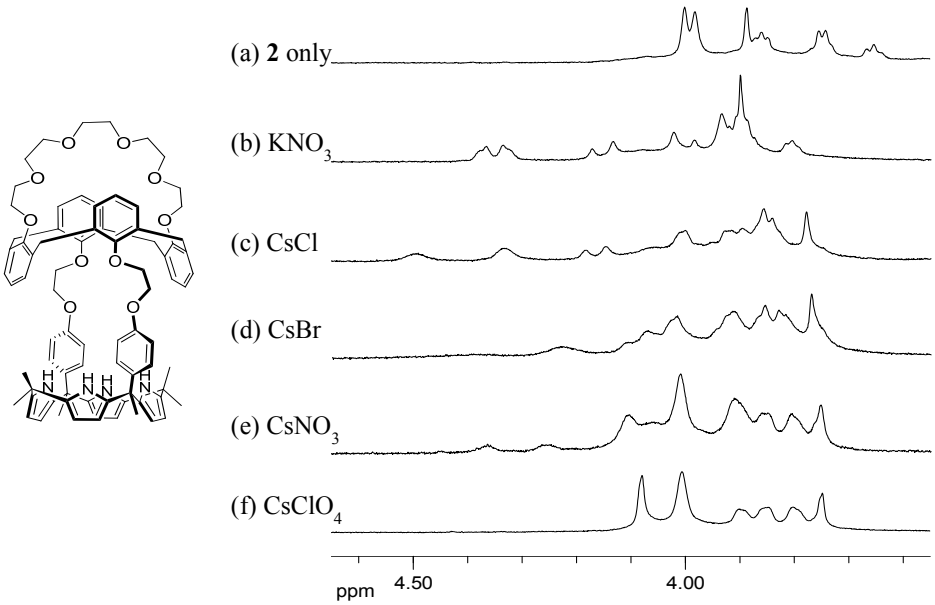

Figure S5. Partial ^{1}H NMR spectra of nitrobenzene-d_5 solutions of **2** after exposure to (a) an ion-free aqueous D_2O solution, (b) an aqueous D_2O solution of KNO_3 (5 equiv), (c) an aqueous D_2O solution of CsCl (5 equiv), (d) an aqueous D_2O solution of CsBr (5 equiv), (e) an aqueous D_2O solution of $CsNO_3$ (5 equiv), and (f) an aqueous D_2O solution of $CsClO_4$ (5 equiv).

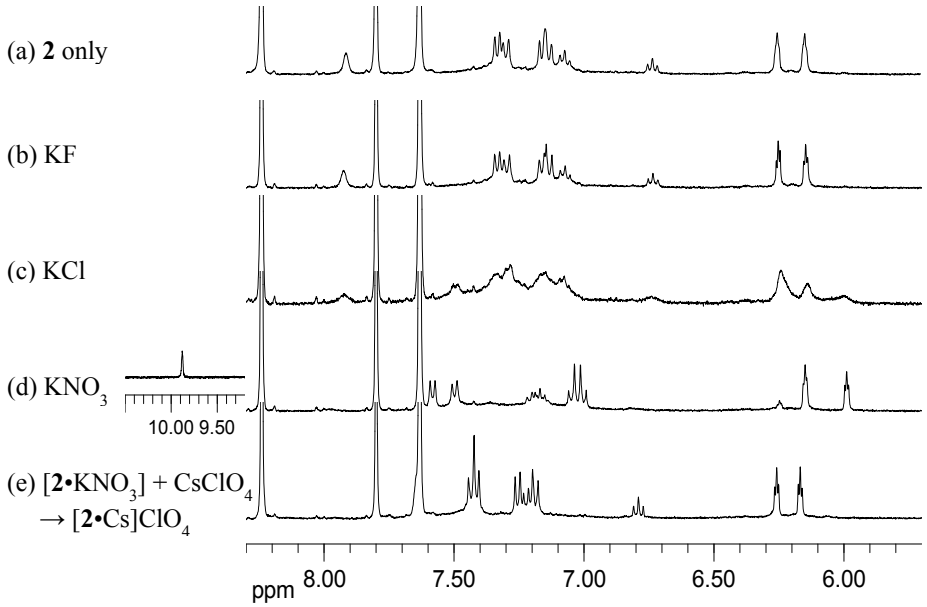

Figure S6. Partial ^{1}H NMR spectra of nitrobenzene-d_5 solutions of **2** (a) after being washed with D_2O, (b) after contacting with an aqueous KF solution (5 equiv), (c) after contacting with an aqueous KCl solution (5 equiv), (d) after contacting with an aqueous KNO_3 solution (5 equiv), and (e) after the nitrobenzene phase obtained from (d) was washed with first D_2O and then an aqueous D_2O $CsClO_4$ solution (5 equiv).

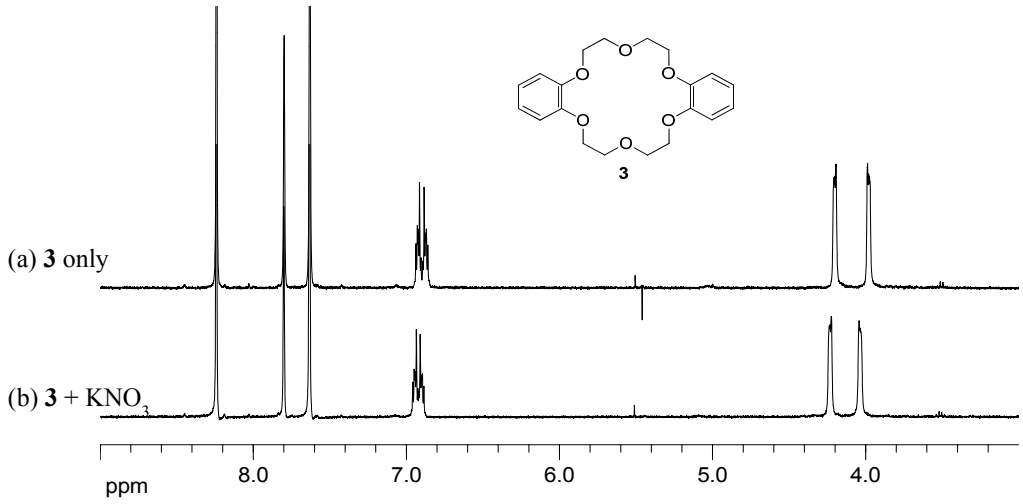

Figure S7. Partial ^{1}H NMR spectra of nitrobenzene-d_5 solutions of **3** (a) after being washed with D_2O and (b) after contacting with an aqueous KNO_3 solution (5 equiv).

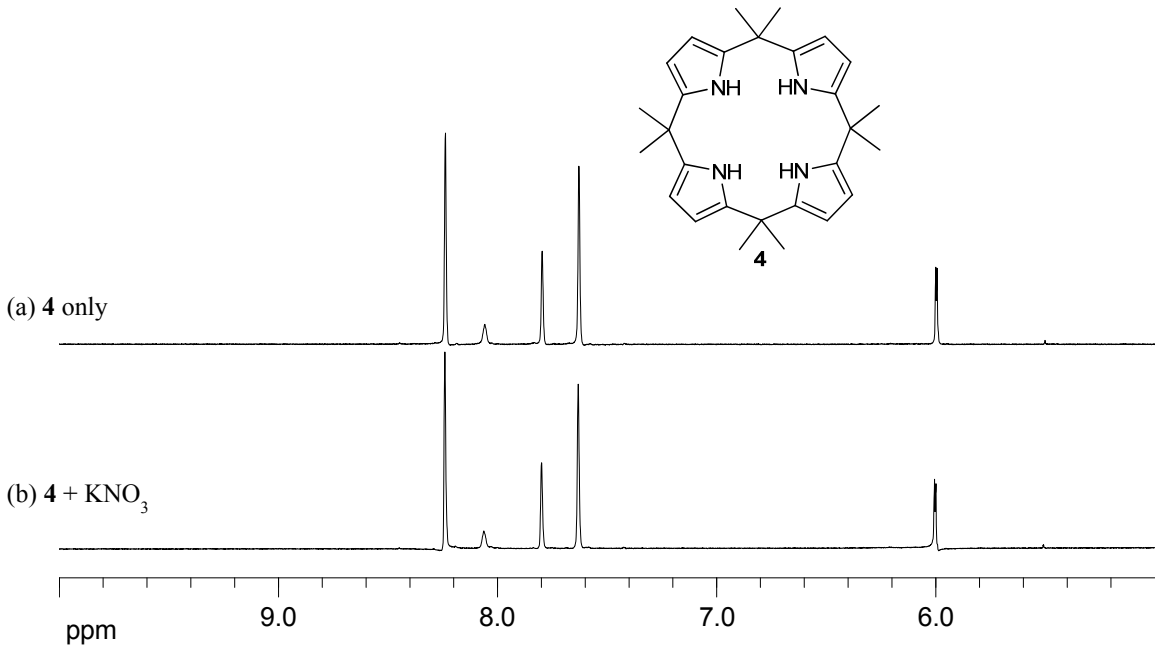

Figure S8. Partial ^{1}H NMR spectra of nitrobenzene-d_5 solutions of **4** (a) after being washed with D_2O and (b) after contacting with an aqueous KNO_3 solution (5 equiv).

Table S1. Calculated Gas-Phase Binding Energy for Ion Pairs and Individual Ions in Different Binding Modes of Receptor **2**, ΔE^a (kcal/mol).

Ion pair	crown/crown	crown/pyrrole	glycol/pyrrole	pyrrole/pyrrole
CsF	-148.3	-125.2	-155.1	-148.2
CsCl	-140	-111.2	-138.9	-125.7
CsBr	-136.4	-104.8	-131.7	-114.5
$CsNO_3$	-130.3	-110.6	-128.2	-104.3
$CsClO_4$	-133.2	-110.1	-123.8	-99.9
KF	-162.5	-140.7	-163.3	-162.2
KCl	-150.1	-128	-150.1	-138.4
KBr	-146.5	-121.9	-146.1	-126.5
KNO_3	-140.3	-119.1	-143.5	-115.9
$KClO_4$	-142.6	-123.1	-141.8	-112

Anion	pyrrole	cation	crown	glycol
F^-	-41.6	K^+	-75.7	-63.6
Cl^-	-26.1	Cs^+	-66.5	-40.9
Br^-	-16.4			
NO_3^-	-13.2			
ClO_4^-	-10.1			

[a] $\Delta E = E(\text{complex}) - E(\text{ligand}) - E(\text{cation}) - E(\text{anion})$.

Supporting info for modeling:

Molecular mechanics calculations were performed using the MMFF94 force field[1] as implemented in PCModel.[2] Non-default van der Waals parameters used for the cesium cation are described elsewhere.[3] Optimized Cartesian coordinates for the four CsF binding modes are provided below.

1. Halgren, T. A. *J. Comp. Chem*. **1996**, *17*, 490-519.
2. PC Model, v9.0, Serena Software, Serena Software, Box 3076, Bloomington, IN 47402-3076.
3. Kim, S. K.; Sessler, J. L.; Gross, D. E.; Lee, C.-H.; Kim, J. S.; Lynch, V. M.; Delmau, L. H.; Hay, B. P. *J. Am. Chem. Soc.* **2010**, *132*, 5827-5836.


```
CsCl crown/pyrrole mode
182
Cs     -0.019      4.928      1.313
Cl     -0.004     -5.078      0.268
O      -1.693      3.574     -1.019
C       2.271      2.210     -0.726
C       3.011      2.799      0.312
C       3.230      4.183      0.255
C       2.641      4.955     -0.750
C       1.756      4.367     -1.658
C       1.528      2.985     -1.632
C       3.570      1.976      1.462
C       1.597      1.769      3.116
C       0.582      1.009      3.733
C       0.572     -0.378      3.513
C       1.515     -0.986      2.690
C       2.489     -0.214      2.063
C       2.538      1.177      2.244
O      -2.205      6.336     -1.248
C      -0.538      1.606      4.573
C      -2.300      1.841      2.746
C      -3.043      2.630      1.851
C      -3.265      3.971      2.193
C      -2.678      4.521      3.336
C      -1.791      3.761      4.104
C      -1.559      2.414      3.792
C      -3.599      2.061      0.556
C      -1.626      2.205     -1.104
C      -2.565      1.443     -0.374
C      -2.512      0.044     -0.484
C      -1.536     -0.578     -1.256
C      -0.595      0.189     -1.936
C      -0.609      1.592     -1.865
O      -1.186      8.324      0.707
C       0.509      2.352     -2.563
O       1.140      8.129      2.607
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C	-3.429	-0.052	3.378
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C	4.477	-8.509	2.115
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C	1.637	-7.138	-3.182
C	-1.639	-7.811	3.218
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CsCl glycol/pyrrole mode
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Cs     -0.011     -1.224      0.159
Cl     -0.086     -4.509      0.187
O       0.181      3.627      2.918
C      -2.634      2.331      0.106
C      -2.524      3.020     -1.120
C      -2.375      4.415     -1.084
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C      -2.490      2.997      1.341
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C      -0.093     -0.577     -3.128
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C	2.689	2.837	-1.220
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C	-1.094	1.580	2.960
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O	-0.173	9.092	-2.441
O	2.964	0.832	0.081
O	4.082	-1.567	-1.083
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C	-2.319	-7.754	-1.729
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H	1.627	-6.175	0.863
H	-0.672	-6.423	1.719
H	-1.879	-6.112	-0.430
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H	-2.644	3.038	-3.280
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H	1.663	5.501	4.046
H	0.537	5.915	5.365

H	1.608	7.589	3.199
H	0.400	8.223	4.359
H	4.883	0.996	0.895
H	4.819	0.892	-0.888
H	3.952	-1.354	0.986
H	5.605	-1.220	0.276
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H	-4.772	1.206	-0.731
H	-4.715	1.165	1.055
H	0.239	-8.886	-4.747
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H	-0.623	-8.677	5.279
H	-3.142	-8.567	4.373
H	-3.982	-9.661	0.405
H	-3.053	-9.792	-2.109
H	-4.722	-8.658	2.459
H	-5.042	-7.117	3.255
H	-5.587	-7.388	1.596
H	1.180	-5.115	2.860
H	1.249	-5.331	4.598
H	2.719	-5.508	3.622
H	1.838	-8.974	4.761
H	3.108	-7.746	4.723
H	1.637	-7.475	5.666
H	-1.195	8.442	2.316
H	0.185	9.585	2.386
H	-1.289	8.748	-0.030
H	0.092	9.852	0.023
H	1.396	8.206	-1.401
H	-0.073	7.220	-1.533
H	0.190	9.641	-4.351
H	1.431	8.578	-3.667
H	-1.444	7.581	-4.069
H	-0.315	7.665	-5.457
H	-1.488	5.190	-4.210
H	-0.470	5.374	-5.666
H	-0.087	3.157	-4.960
H	1.351	4.070	-4.422
H	4.337	-8.964	-1.926
H	5.265	-7.708	-1.111
H	4.732	-7.471	-2.779
H	-1.382	-5.151	-2.463
H	-2.939	-5.494	-3.212
H	-1.464	-5.427	-4.192
H	-2.233	-9.040	-4.221
H	-1.958	-7.586	-5.182
H	-3.440	-7.749	-4.230
H	-4.789	-5.593	-0.180
H	-5.107	-3.209	-0.425
H	-3.027	-2.543	3.292
H	-2.694	-4.945	3.541
H	4.561	-5.811	0.596

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H       4.998      -3.439       0.753
H       2.946      -2.807      -2.986
H       2.493      -5.197      -3.146

CsCl crown/crown mode
182
Cs      0.387       6.266      -0.110
Cl      2.390       8.766       0.499
O       0.296       4.077       2.646
C      -2.414       2.614       0.018
C      -2.459       3.280      -1.223
C      -2.755       4.653      -1.231
C      -2.936       5.351      -0.039
C      -2.769       4.700       1.182
C      -2.482       3.328       1.230
C      -2.219       2.582      -2.549
C       0.346       2.442      -2.641
C       1.534       1.684      -2.647
C       1.430       0.296      -2.836
C       0.191      -0.331      -2.943
C      -0.973       0.421      -2.846
C      -0.917       1.814      -2.676
O      -0.792       6.720       3.257
C       2.925       2.273      -2.470
C       3.040       2.480       0.086
C       3.136       3.263       1.254
C       3.541       4.601       1.122
C       3.790       5.152      -0.133
C       3.583       4.394      -1.282
C       3.171       3.056      -1.193
C       2.860       2.728       2.648
C       0.295       2.707       2.762
C       1.528       2.028       2.843
C       1.519       0.650       3.110
C       0.319      -0.040       3.246
C      -0.889       0.633       3.083
C      -0.925       2.009       2.806
O      -1.631       8.599       1.131
C      -2.276       2.665       2.581
O      -1.704       8.550      -1.826
O       2.797       1.132       0.172
O       3.736      -1.482      -1.087
O      -0.189       6.533      -3.436
O       0.375       3.815      -2.596
N      -0.597      -7.618      -1.734
C       0.245       4.659       3.964
C       0.388       6.173       3.857
C      -0.786       8.151       3.342
C      -1.929      -7.410      -2.023
O      -3.364      -1.177       1.558
C       4.026       0.410       0.369
C       3.731      -1.088       0.293
C      -3.354      -0.902       0.150
C      -3.548       0.601      -0.049
C      -1.972      -6.438      -3.005
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C	-0.644	-6.039	-3.281
C	0.204	-6.760	-2.456
N	2.451	-7.314	0.059
C	2.195	-7.711	-1.236
C	2.410	-9.079	-1.273
C	2.754	-9.506	0.031
C	2.750	-8.398	0.856
N	0.633	-7.471	2.701
C	1.976	-7.313	2.974
C	2.076	-6.265	3.870
C	0.772	-5.772	4.109
C	-0.117	-6.513	3.347
N	-2.395	-7.145	0.882
C	-2.161	-7.449	2.206
C	-2.454	-8.795	2.354
C	-2.824	-9.306	1.089
C	-2.758	-8.271	0.175
C	-2.088	-4.982	2.761
C	-2.224	-6.728	4.614
C	4.441	-7.643	2.514
C	2.980	-9.585	3.077
C	2.255	-5.297	-1.988
C	-1.939	8.724	2.523
C	-2.447	9.443	0.315
C	-1.716	9.721	-0.996
C	-0.935	8.800	-3.011
C	-1.011	7.594	-3.942
C	-0.184	5.419	-4.335
C	0.808	4.364	-3.854
C	2.296	-7.191	-3.693
C	-4.408	-7.561	-1.542
C	-3.060	-9.622	-1.941
C	3.021	-8.226	2.345
C	-1.643	-6.407	3.206
C	1.734	-6.727	-2.319
C	-3.022	-8.207	-1.323
C	-3.379	-4.497	3.047
C	-3.790	-3.230	2.622
C	-2.934	-2.435	1.869
C	-1.657	-2.889	1.560
C	-1.245	-4.155	1.988
C	3.570	-4.906	-2.307
C	4.048	-3.633	-1.983
C	3.238	-2.736	-1.298
C	1.938	-3.094	-0.958
C	1.459	-4.367	-1.285
O	-2.269	1.250	0.064
H	-0.260	-8.290	-1.054
H	2.389	-6.361	0.398
H	0.258	-8.179	2.081
H	-2.278	-6.228	0.467
H	-2.832	5.197	-2.170
H	-3.164	6.414	-0.061
H	-2.852	5.277	2.101
H	-2.253	3.306	-3.371

H	-3.073	1.921	-2.743
H	2.327	-0.316	-2.885
H	0.141	-1.408	-3.076
H	-1.932	-0.089	-2.897
H	3.681	1.478	-2.511
H	3.138	2.895	-3.348
H	3.667	5.235	1.998
H	4.117	6.188	-0.213
H	3.751	4.862	-2.249
H	3.686	2.061	2.925
H	2.917	3.543	3.380
H	2.453	0.101	3.203
H	0.320	-1.107	3.452
H	-1.815	0.069	3.165
H	-3.081	1.930	2.709
H	-2.438	3.390	3.388
H	1.063	4.273	4.584
H	-0.712	4.418	4.440
H	1.254	6.433	3.238
H	0.515	6.594	4.861
H	0.168	8.538	2.970
H	-0.909	8.433	4.393
H	4.424	0.636	1.363
H	4.764	0.691	-0.392
H	2.773	-1.300	0.780
H	4.529	-1.642	0.800
H	-4.197	-1.440	-0.300
H	-2.422	-1.220	-0.329
H	-3.954	0.770	-1.052
H	-4.248	0.997	0.697
H	-2.865	-6.051	-3.479
H	-0.332	-5.290	-3.998
H	2.307	-9.712	-2.146
H	2.973	-10.523	0.332
H	2.990	-5.889	4.310
H	0.505	-4.949	4.760
H	-2.386	-9.359	3.276
H	-3.101	-10.330	0.871
H	-1.796	-7.652	5.024
H	-2.005	-5.928	5.332
H	-3.310	-6.872	4.596
H	4.526	-6.646	2.064
H	4.717	-7.551	3.571
H	5.192	-8.281	2.032
H	2.011	-10.084	2.950
H	3.753	-10.268	2.706
H	3.142	-9.460	4.155
H	-2.872	8.185	2.721
H	-2.059	9.780	2.788
H	-3.399	8.934	0.137
H	-2.632	10.399	0.816
H	-2.234	10.523	-1.534
H	-0.684	10.028	-0.789
H	-1.350	9.674	-3.525
H	0.105	8.996	-2.729

H	-2.044	7.236	-4.020
H	-0.645	7.884	-4.933
H	-1.195	5.005	-4.388
H	0.117	5.760	-5.332
H	0.916	3.599	-4.634
H	1.781	4.837	-3.688
H	1.818	-8.121	-4.030
H	3.373	-7.392	-3.660
H	2.120	-6.441	-4.475
H	-4.434	-6.527	-1.176
H	-5.192	-8.114	-1.011
H	-4.681	-7.541	-2.603
H	-2.120	-10.163	-1.772
H	-3.217	-9.577	-3.026
H	-3.869	-10.227	-1.517
H	-4.094	-5.098	3.604
H	-4.781	-2.867	2.882
H	-0.960	-2.255	1.019
H	-0.242	-4.481	1.718
H	4.251	-5.587	-2.812
H	5.057	-3.345	-2.267
H	1.277	-2.384	-0.471
H	0.441	-4.616	-0.993

CsCl pyrrole/pyrrole mode
182

Cs	0.355	-9.524	0.078
Cl	0.163	-5.108	0.034
O	-3.111	3.365	0.601
C	-0.794	2.229	-2.810
C	0.396	2.973	-2.901
C	0.322	4.367	-2.754
C	-0.889	4.991	-2.466
C	-2.037	4.227	-2.274
C	-2.000	2.832	-2.414
C	1.754	2.305	-3.023
C	2.583	2.295	-0.601
C	2.745	1.633	0.631
C	2.650	0.231	0.655
C	2.353	-0.486	-0.501
C	2.112	0.191	-1.694
C	2.196	1.591	-1.758
O	-3.966	6.050	0.405
C	2.864	2.378	1.948
C	0.442	2.341	2.761
C	-0.821	2.952	2.847
C	-0.896	4.343	2.690
C	0.239	5.094	2.388
C	1.462	4.458	2.197
C	1.576	3.069	2.356
C	-2.101	2.145	2.980
C	-2.914	2.010	0.556
C	-2.473	1.366	1.729
C	-2.273	-0.023	1.697
C	-2.454	-0.743	0.518

C	-2.809	-0.079	-0.654
C	-3.020	1.310	-0.661
O	-1.479	7.789	0.364
C	-3.204	2.010	-1.996
O	1.739	9.034	-0.844
O	0.554	0.993	2.992
O	1.929	-1.403	4.106
O	3.626	6.431	-0.773
O	2.708	3.660	-0.679
N	2.601	-6.972	0.813
C	-4.497	3.708	0.719
C	-4.591	5.121	1.296
C	-3.770	7.332	1.009
C	3.381	-7.633	-0.123
O	-1.917	-1.651	-4.102
C	0.861	0.747	4.373
C	0.762	-0.756	4.626
C	-0.808	-0.913	-4.629
C	-1.039	0.579	-4.401
C	4.021	-8.655	0.555
C	3.608	-8.620	1.904
C	2.711	-7.577	2.057
N	-0.495	-7.108	2.412
C	0.502	-7.705	3.170
C	-0.056	-8.844	3.723
C	-1.394	-8.938	3.282
C	-1.659	-7.857	2.458
N	-2.104	-7.192	-0.707
C	-2.824	-7.899	0.243
C	-3.372	-8.988	-0.414
C	-2.962	-8.943	-1.763
C	-2.159	-7.829	-1.938
N	0.994	-7.090	-2.305
C	0.053	-7.786	-3.051
C	0.709	-8.883	-3.582
C	2.050	-8.852	-3.140
C	2.219	-7.736	-2.337
C	-1.534	-5.785	-3.434
C	-2.042	-7.943	-4.459
C	-3.220	-5.946	1.825
C	-4.161	-8.145	2.369
C	1.908	-5.566	3.513
C	-2.841	8.176	0.135
C	-0.573	8.570	-0.414
C	0.868	8.121	-0.173
C	3.125	8.800	-0.571
C	3.709	7.691	-1.447
C	4.146	5.372	-1.587
C	4.081	4.040	-0.841
C	2.602	-7.652	4.580
C	3.607	-5.684	-1.744
C	4.736	-7.804	-2.245
C	-2.932	-7.460	1.706
C	-1.409	-7.313	-3.183
C	1.917	-7.104	3.292

C	3.452	-7.215	-1.594
C	-0.583	-5.111	-4.227
C	-0.676	-3.737	-4.479
C	-1.731	-2.999	-3.953
C	-2.716	-3.658	-3.218
C	-2.628	-5.034	-2.972
C	0.903	-4.963	4.297
C	0.876	-3.583	4.524
C	1.861	-2.764	3.981
C	2.898	-3.348	3.255
C	2.931	-4.730	3.034
O	-0.759	0.874	-3.024
H	1.997	-6.167	0.615
H	-0.367	-6.247	1.869
H	-1.572	-6.334	-0.526
H	0.791	-6.233	-1.779
H	1.222	4.973	-2.800
H	-0.926	6.064	-2.309
H	-2.946	4.724	-1.942
H	2.519	3.042	-3.301
H	1.735	1.604	-3.867
H	2.735	-0.309	1.595
H	2.228	-1.566	-0.451
H	1.794	-0.383	-2.560
H	3.174	1.692	2.746
H	3.684	3.101	1.888
H	-1.853	4.852	2.735
H	0.147	6.163	2.223
H	2.312	5.045	1.857
H	-2.007	1.464	3.836
H	-2.939	2.802	3.248
H	-1.913	-0.548	2.576
H	-2.241	-1.810	0.493
H	-2.847	-0.646	-1.582
H	-3.428	1.277	-2.781
H	-4.102	2.637	-1.962
H	-5.025	3.011	1.382
H	-4.960	3.690	-0.272
H	-4.091	5.147	2.270
H	-5.640	5.407	1.426
H	-3.333	7.215	2.007
H	-4.748	7.818	1.090
H	0.136	1.261	5.016
H	1.871	1.104	4.601
H	-0.142	-1.138	4.137
H	0.717	-0.936	5.706
H	-0.744	-1.106	-5.706
H	0.123	-1.207	-4.132
H	-0.360	1.144	-5.051
H	-2.076	0.843	-4.639
H	4.728	-9.355	0.127
H	3.942	-9.291	2.686
H	0.443	-9.535	4.390
H	-2.099	-9.714	3.554
H	-4.015	-9.737	0.029

H	-3.235	-9.656	-2.531
H	0.272	-9.628	-4.235
H	2.819	-9.569	-3.397
H	-2.022	-9.039	-4.439
H	-3.092	-7.645	-4.575
H	-1.513	-7.636	-5.371
H	-2.437	-5.322	1.392
H	-4.152	-5.679	1.311
H	-3.318	-5.644	2.875
H	-4.088	-9.239	2.351
H	-4.264	-7.847	3.420
H	-5.092	-7.877	1.855
H	-3.081	8.038	-0.925
H	-2.951	9.231	0.406
H	-0.813	8.478	-1.480
H	-0.677	9.628	-0.144
H	1.079	8.120	0.902
H	1.013	7.103	-0.551
H	3.631	9.737	-0.825
H	3.281	8.612	0.497
H	3.177	7.633	-2.403
H	4.769	7.903	-1.630
H	3.562	5.315	-2.512
H	5.190	5.595	-1.833
H	4.639	3.288	-1.415
H	4.537	4.153	0.147
H	2.677	-8.745	4.581
H	2.047	-7.374	5.486
H	3.622	-7.261	4.689
H	2.773	-5.122	-1.323
H	3.680	-5.395	-2.800
H	4.512	-5.327	-1.236
H	4.759	-8.899	-2.205
H	5.640	-7.445	-1.737
H	4.813	-7.519	-3.301
H	0.256	-5.651	-4.661
H	0.097	-3.281	-5.087
H	-3.554	-3.094	-2.816
H	-3.429	-5.499	-2.403
H	0.115	-5.567	4.743
H	0.067	-3.184	5.125
H	3.683	-2.720	2.840
H	3.769	-5.134	2.471