Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Elucidating the Structures and Cooperative Binding Mechanism of Cesium Salts to Multi-topic Ion-Pair Receptor through Density Functional Theory Calculation

*Biswajit Sadhu,[(1)]Mahesh Sundararajan,[(2)]*Gunasekaran Velmurugan[(3)] and Ponnambalam Venuvanalingam[(3)]**

[1] Radiation Safety Systems Division, [2] Theoretical Chemistry Section,

Bhabha Atomic Research Centre, Mumbai– 400085,India.

[3]School of Chemistry, Bharathidasan University, Tiruchirappalli-620024

TableS1. Optimized geometric parameters (Å) of Receptor-$Cs^{+}Cl^{-}$ complex in C/P binding mode at various levels.

Optimization Level	Medium	Cs-O_C	Cs-C_A	Cl-N_P	RMSD[a]
BP86/B1	ε=80	2.94-3.12	3.44-3.45	3.21-3.23	0.26
BP86-D3/B1	ε=80	2.96-3.17	3.42-3.56	3.19-3.23	0.39
BP86/B2	ε=80	2.93-3.13	3.48-3.53	3.25-3.27	0.26
BP86/B1	ε=1	2.88-3.15	3.45-3.50	3.23-3.25	0.34
BP86-D3/B1	ε=1	2.89-3.19	3.44-3.52	3.21-3.27	0.56
X-ray	-	2.84-3.10	3.29-3.40	3.22-3.30	-

[a]RMSD values are calculated with respect to X-ray structures.

Table S2. Computed binding affinities (kcal mol^{-1}) of CsCl in Receptor at C/P binding mode.

DFT level for energetics	Medium	Binding affinity
B3LYP-D3/B2//BP86/B1	ε=80	-28.67
B3LYP-D3/B2//BP86/B2	ε=80	-32.28

Table S3: Hydration free energy (kcal mol^{-1}) of ions calculated at B3LYP-D3/B2//BP86/B1 level

Hydrated ion	Hydration free energy	
	Calculated	Experimental[a]
$Cs(H_2O)_6^+$	-71.43	-59.80
$F^-(H_2O)_6^-$	-120.55	-111.24
$Cl.(H_2O)_6^-$	-79.79	-81.34
$Br.(H_2O)_6^-$	-69.88	-75.36
$I(H_2O)_6^-$	-66.63	-65.79
$NO_3(H_2O)_6^-$	-70.36	-71.77

[a]experimental values are taken from ref no. 59

Table S4.
Optimized geometric parameters (Å) and binding affinities (kcal mol^{-1}) of Receptor-$Cs^{+}Cl^{-}$ .H_2O complexes.

Receptor.$Cs^{+}Cl^{-}.H_2O$	Epsilon (ε)	Cs-$O_{C/G}$	Cs-C_A	Cs-N_P	Cl-N_P	Binding energy
		BP86/B1				B3LYP-D3/B2//BP86/B1
G/P	80	3.10-4.47	3.39-3.55	-	3.25-3.27	-29.45
	5.5	3.10-4.57	3.38-3.57	-	3.26-3.30	-44.95
C/P	80	2.92-3.11	3.45-3.51	-	3.23-3.26	-32.62
	5.5	2.91-3.12	3.45-3.52	-	3.24-3.27	-45.28
	Exp[a]	2.84-3.10	3.29-3.40	-	3.23-3.31	-
P/P	80	-	-	3.53-3.58	3.24-3.29	-29.57
	5.5	-	-	3.46-3.51	3.24-3.28	-37.91

[a]Experimental values are taken from ref. no 25

Table S5.

Topological properties of Receptor-Cs^+F^- (C/P) computed at BP86/B2 level. ρ(r) in units of $eÅ^{-3}$, L(r) in units of $eÅ^{-3}$, G(r), V(r), H(r) in units of a.u. $Å^{-3}$.

Receptor-Cs^+F^- (C/P)							
BCP	ρ(r)	L(r)	G(r)	H(r)	ε	V(r)	-V(r)/G(r)
N-H···F	0.0461	-0.0353	0.0403	-0.0050	0.0204	0.0453	-1.1241
N-H···F	0.0465	-0.0357	0.0408	-0.0050	0.0199	0.0458	-1.1225
N-H···F	0.0443	-0.0338	0.0386	-0.0048	0.0207	0.0435	-1.1269
N-H···F	0.0442	-0.0337	0.0385	-0.0048	0.0215	0.0433	-1.1247
C-H···F	0.0058	-0.0062	0.0048	0.0014	0.1974	0.0034	-0.7083
C-H···F	0.0073	-0.0076	0.0062	0.0014	0.0939	0.0048	-0.7742
C-H···F	0.0054	-0.0056	0.0042	0.0013	0.0625	0.0029	-0.6905
O···Cs	0.0199	-0.0172	0.0160	0.0011	0.1329	0.0149	-0.9313
O···Cs	0.0149	-0.1219	0.0114	0.0008	0.0795	0.0106	-0.9298
O···Cs	0.0163	-0.0136	0.0126	0.0009	0.0847	0.0117	-0.9286
O···Cs	0.0149	-0.0122	0.0114	0.0008	0.0789	0.0106	-0.9298
O···Cs	0.0201	-0.0175	0.0163	0.0011	0.1338	0.0152	-0.9325
C_π···Cs	0.0094	-0.0075	0.0062	0.0013	3.1113	0.0049	-0.7903
C_π···Cs	0.0093	-0.0076	0.0062	0.0013	2.8472	0.0049	-0.7903

Table S6.

Topological properties of Receptor-$Cs^{+}Cl^{-}$ (C/P) computed at BP86/B2 level. ρ(r) in units of $eÅ^{-3}$, L(r) in units of $eÅ^{-3}$, G(r), V(r), H(r) in units of a.u. $Å^{-3}$.

Receptor-$Cs^{+}Cl^{-}$ (C/P)							
BCP	ρ(r)	L(r)	G(r)	H(r)	ε	V(r)	-V(r)/G(r)
N-H···Cl	0.0277	-0.0189	0.0202	-0.0014	0.0129	0.0216	-1.0693
N-H···Cl	0.0282	-0.0191	0.0206	-0.0015	0.0135	0.0221	-1.0728
N-H···Cl	0.0269	-0.0184	0.0194	-0.0011	0.0142	0.0206	-1.0619
N-H···Cl	0.0269	-0.0185	0.0197	-0.0012	0.0149	0.0209	-1.0609
C-H···Cl	0.0094	-0.0076	0.0062	0.0013	0.0081	0.0049	-0.7903
C-H···Cl	0.0090	-0.0072	0.0059	0.0013	0.0135	0.0046	-0.7797
C-H···Cl	0.0095	-0.0077	0.0064	0.0013	0.0137	0.0050	-0.7813
C_{π}···Cl	0.0039	-0.0028	0.0023	0.0005	0.8139	0.0018	-0.7826
C_{π}···Cl	0.0042	-0.0030	0.0025	0.0005	0.1235	0.0019	-0.7600
O···Cs	0.0189	-0.0164	0.0152	0.0011	0.1349	0.0141	-0.9276
O···Cs	0.0141	-0.0115	0.0107	0.0008	0.0713	0.0099	-0.9252
O···Cs	0.0154	-0.0128	0.0118	0.0009	0.0904	0.0109	-0.9237
O···Cs	0.0141	-0.0115	0.0107	0.0008	0.0724	0.0099	-0.9252
O···Cs	0.0191	-0.0163	0.0152	0.0011	0.1329	0.0141	-0.9276
C_{π}···Cs	0.0093	-0.0076	0.0062	0.0013	5.4798	0.0049	-0.7903
C_{π}···Cs	0.0091	-0.0074	0.0061	0.0013	2.2582	0.0047	-0.7705

Table S7.

Topological properties of Receptor-$Cs^{+}Br^{-}$ (G/P) computed at BP86/B2 level. ρ(r) in units of $eÅ^{-3}$, L(r) in units of $eÅ^{-3}$, G(r), V(r), H(r) in units of a.u. $Å^{-3}$.

Receptor-$Cs^{+}Br^{-}$ (G/P)							
BCP	ρ(r)	L(r)	G(r)	H(r)	ε	V(r)	-V(r)/G(r)
N-H···Br	0.0190	-0.0127	0.0124	0.0003	0.0275	0.0120	-0.9677
N-H···Br	0.0192	-0.0128	0.0125	0.0003	0.0269	0.0122	-0.9760
N-H···Br	0.0182	-0.0123	0.0119	0.0004	0.0302	0.0114	-0.9580
N-H···Br	0.0180	-0.0121	0.0117	0.0004	0.0310	0.0112	-0.9573
C-H···Br	0.0095	-0.0067	0.0056	0.0010	0.0211	0.0046	-0.8214
C-H···Br	0.0091	-0.0064	0.0054	0.0010	0.0234	0.0043	-0.7963
C-H···Br	0.0033	-0.0023	0.0018	0.0005	0.6375	0.0013	-0.7222
C_{π}···Br	0.0043	-0.0029	0.0024	0.0005	1.3654	0.0019	-0.7917
C_{π}···Br	0.0042	-0.0028	0.0023	0.0005	1.3723	0.0019	-0.8261
Cs···Br	0.0060	-0.0040	0.0033	0.0007	0.0015	0.0025	-0.7576
C-H···Cs	0.0032	-0.0029	0.0021	0.0008	0.2691	0.0014	-0.6667
C-H···Cs	0.0032	-0.0029	0.0021	0.0008	0.3960	0.0014	-0.6667
O···Cs	0.0079	-0.0071	0.0061	0.0010	0.1100	0.0051	-0.8361
O···Cs	0.0089	-0.0079	0.0069	0.0010	0.1152	0.0059	-0.8551
C_{π}···Cs	0.0067	-0.0049	0.0040	0.0009	0.6206	0.0030	-0.7500
C_{π}···Cs	0.0089	-0.0071	0.0058	0.0013	2.4049	0.0045	-0.7759

Table S8.

Topological properties of Receptor-$Cs^{+}I^{-}$ (G/P) computed at BP86/B2 level. ρ(r) in units of $eÅ^{-3}$, L(r) in units of $eÅ^{-3}$, G(r), V(r), H(r) in units of a.u. $Å^{-3}$.

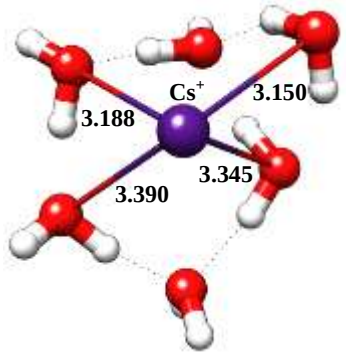
Receptor-$Cs^{+}I^{-}$ (G/P)							
BCP	ρ(r)	L(r)	G(r)	H(r)	ε	V(r)	-V(r)/G(r)
N-H···I	0.0162	-0.0094	0.0095	-0.0001	0.0149	0.0095	-1.0000
N-H···I	0.0162	-0.0095	0.0095	-0.0001	0.0152	0.0095	-1.0000
N-H···I	0.0148	-0.0089	0.0087	0.0002	0.0197	0.0085	-0.9770
N-H···I	0.0147	-0.0089	0.0086	0.0002	0.0188	0.0084	-0.9767
C-H···I	0.0087	-0.0057	0.0048	0.0009	0.0220	0.0039	-0.8125
C-H···I	0.0093	-0.0061	0.0052	0.0009	0.0199	0.0043	-0.8269
C-H···I	0.0050	-0.0034	0.0026	0.0007	0.4325	0.0019	-0.7308
C_{π}···I	0.0051	-0.0031	0.0026	0.0005	2.1084	0.0021	-0.8077
C_{π}···I	0.0050	-0.0030	0.0025	0.0005	1.8963	0.0020	-0.8000
Cs···I	0.0073	-0.0047	0.0039	0.0008	0.0038	0.0030	-0.7692
C-H···Cs	0.0031	-0.0029	0.0021	0.0008	0.7412	0.0013	-0.6190
O···Cs	0.0022	-0.0023	0.0017	0.0006	0.3557	0.0011	-0.6471
O···Cs	0.0109	-0.0094	0.0084	0.0010	0.1234	0.0074	-0.8810
O···Cs	0.0118	-0.0101	0.0091	0.0010	0.1270	0.0081	-0.8901
C_{π}···Cs	0.0076	-0.0057	0.0047	0.0011	1.0105	0.0036	-0.7660
C_{π}···Cs	0.0082	-0.0067	0.0054	0.0013	8.2469	0.0042	-0.7778

Table S9.

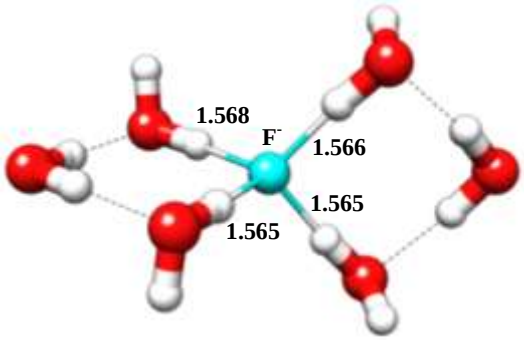
Topological propertiesof Receptor-$Cs^{+}NO_3^{-}$ (G/P) computed at BP86/B2 level. ρ(r) in units of $eÅ^{-3}$, L(r) in units of $eÅ^{-3}$, G(r), V(r), H(r) in units of a.u. $Å^{-3}$.

Receptor-$Cs^{+}NO_3^{-}$ (G/P)							
BCP	ρ(r)	L(r)	G(r)	H(r)	ε	V(r)	-V(r)/G(r)
N-H···O	0.0282	-0.0217	0.0227	-0.0009	0.0592	0.0237	-1.0441
N-H···O	0.0283	-0.0219	0.0229	-0.0009	0.0604	0.0238	-1.0393
N-H···O	0.0258	-0.0199	0.0208	-0.0009	0.0631	0.0216	-1.0385
N-H···O	0.0259	-0.0200	0.0209	-0.0009	0.0639	0.0217	-1.0383
C-H···O	0.0041	-0.0041	0.0031	0.0009	1.3171	0.0021	-0.6774
C_π···O	0.0036	-0.0034	0.0027	0.0007	4.3269	0.0019	-0.7037
C_π···O	0.0036	-0.0034	0.0027	0.0007	4.2951	0.0019	-0.7037
C-H···O	0.0086	-0.0070	0.0063	0.0008	0.0047	0.0055	-0.8730
C_π···O	0.0029	-0.0027	0.0021	0.0006	0.3554	0.0016	-0.7619
C_π···O	0.0029	-0.0028	0.0022	0.0006	0.4010	0.0016	-0.7273
Cs···O	0.0101	-0.0084	0.0075	0.0009	0.0105	0.0065	-0.8667
C-H···O	0.0066	-0.0057	0.0048	0.0009	0.0224	0.0039	-0.8125
C-H···O	0.0029	-0.0028	0.0022	0.0006	1.2024	0.0016	-0.7273
C_π···O	0.0033	-0.0030	0.0024	0.0006	0.5377	0.0018	-0.7500
C_π···O	0.0032	-0.0029	0.0024	0.0006	0.4289	0.0018	-0.7500
Cs···O	0.0102	-0.0086	0.0076	0.0009	0.0219	0.0066	-0.8684
O···Cs	0.0047	-0.0047	0.0038	0.0009	0.0936	0.0028	-0.7368
O···Cs	0.0096	-0.0085	0.0074	0.0009	0.1138	0.0065	-0.8784
O···Cs	0.0102	-0.0089	0.0079	0.0009	0.1169	0.0069	-0.8734
O···Cs	0.0050	-0.0049	0.0040	0.0009	0.0662	0.0031	-0.7750
C_π···Cs	0.0059	-0.0044	0.0036	0.0009	0.7242	0.0027	-0.7500
C_π···Cs	0.0084	-0.0068	0.0055	0.0013	3.0972	0.0042	-0.7636

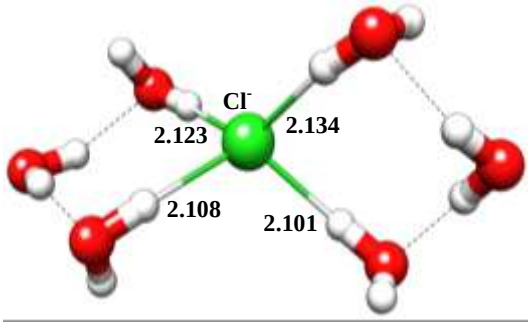
Figure S1: Optimized structures of hydrated ion systems.



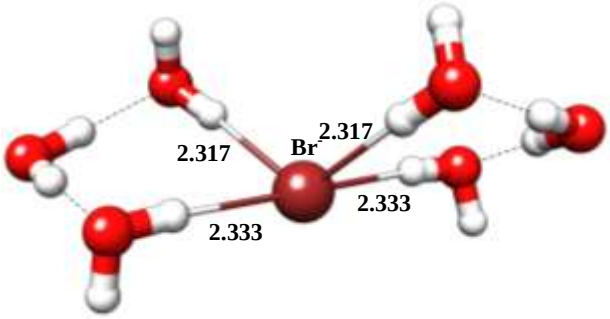
$Cs(H_2O)_6^+$



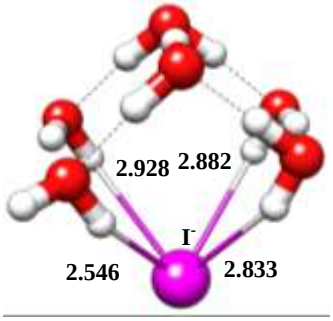
$F(H_2O)_6^-$



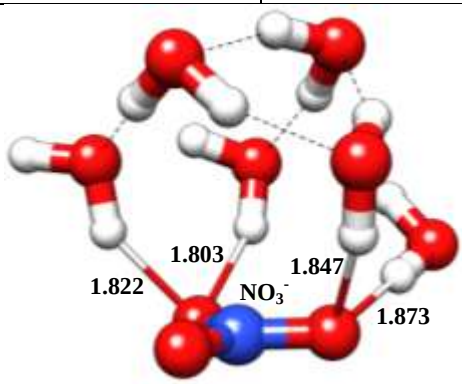
$Cl(H_2O)_6^-$



$Br(H_2O)_6^-$

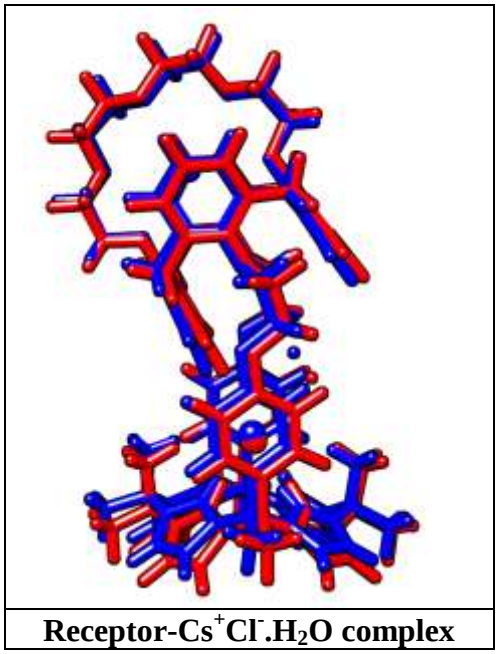


$I(H_2O)_6^-$



$NO_3(H_2O)_6^-$

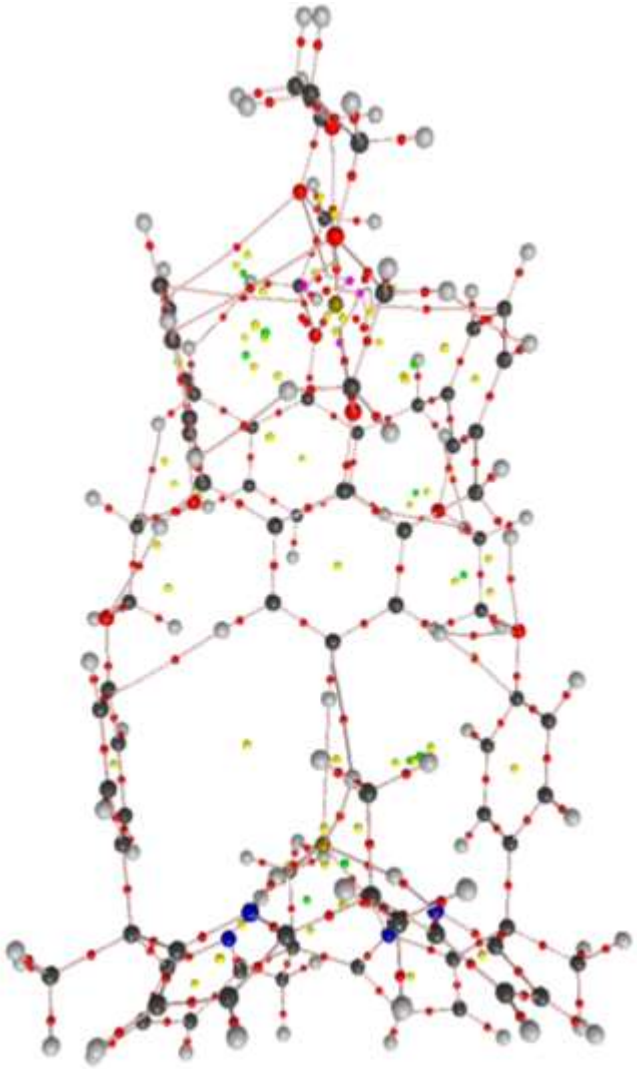
Figure S2: Superimposition of optimized structures (red) and crystal structures (blue) of Receptor-$Cs^{+}Cl^{-}.H_2O$ complex.



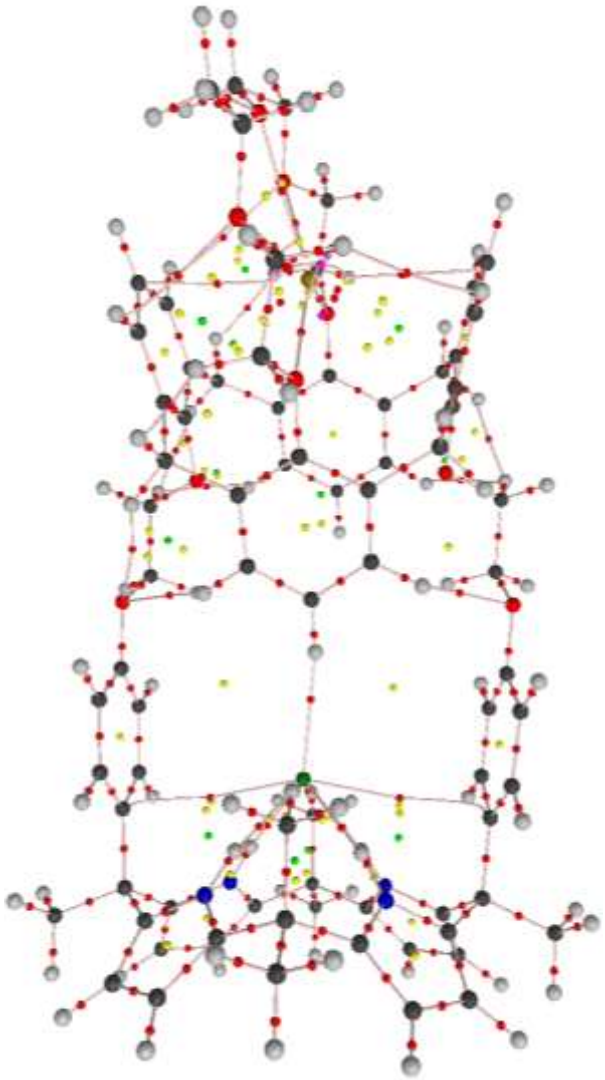
Receptor-$Cs^{+}Cl^{-}.H_2O$ complex

Figure S3: Molecular graphs of the titled cases computed at BP86/B2 showing bond paths, bond critical points in red (BCPs) and ring critical points (RCPs) in yellow.

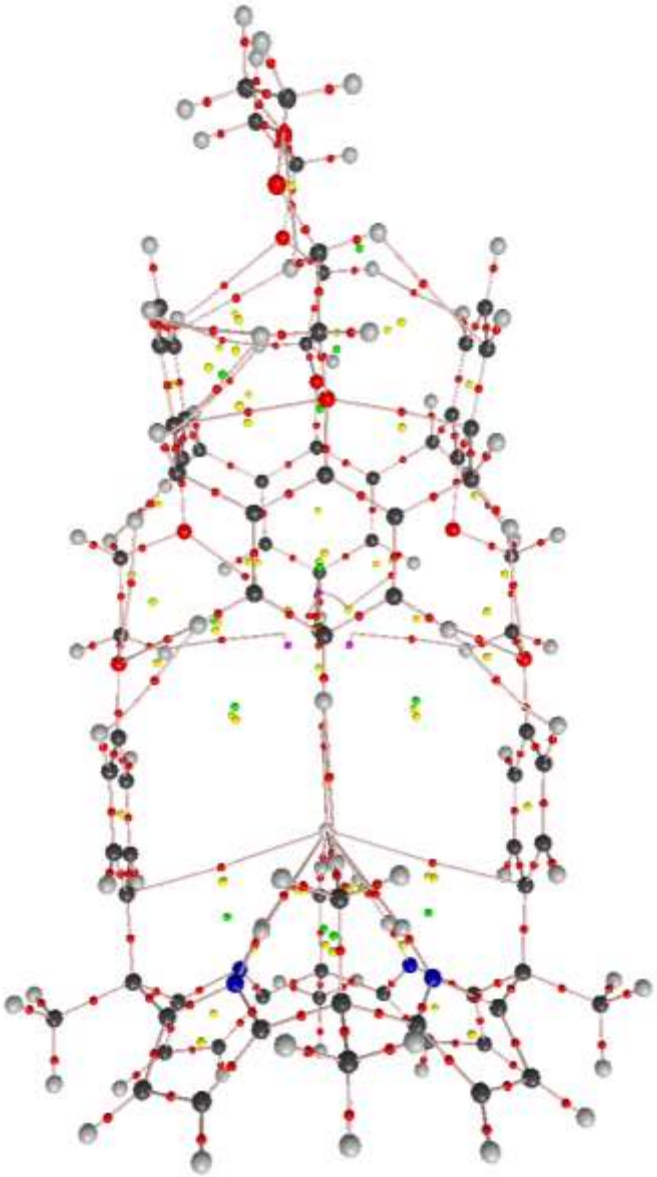
(a) Receptor-$Cs^{+}F^{-}$ (C/P)



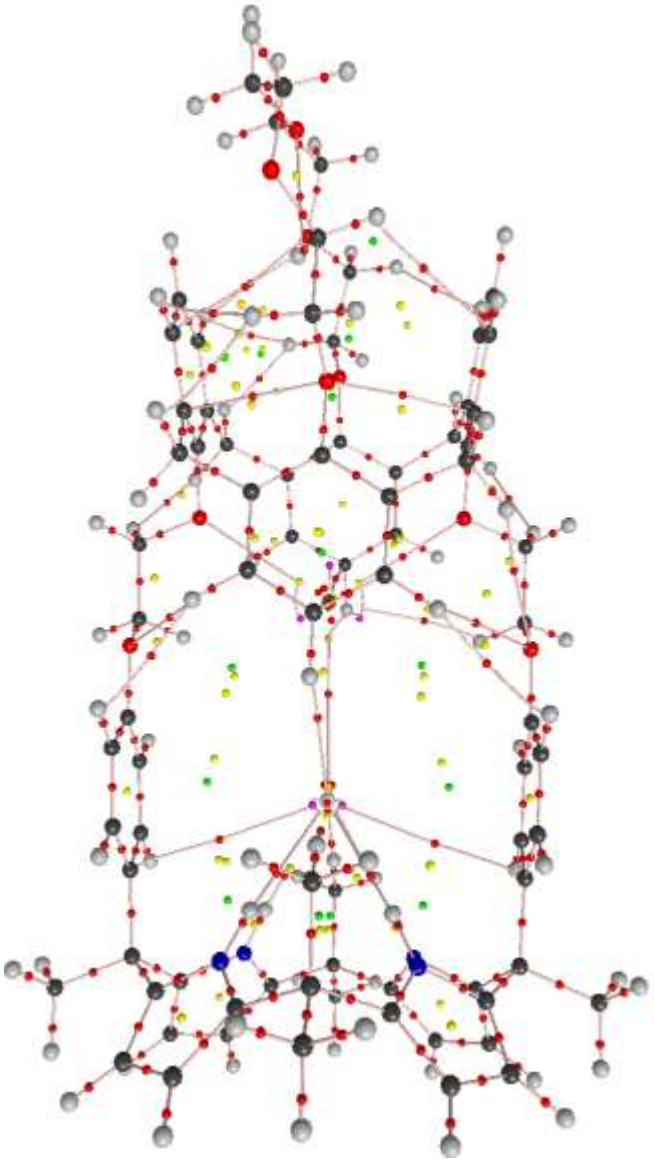
(b) Receptor-$Cs^{+}Cl^{-}$ (C/P)



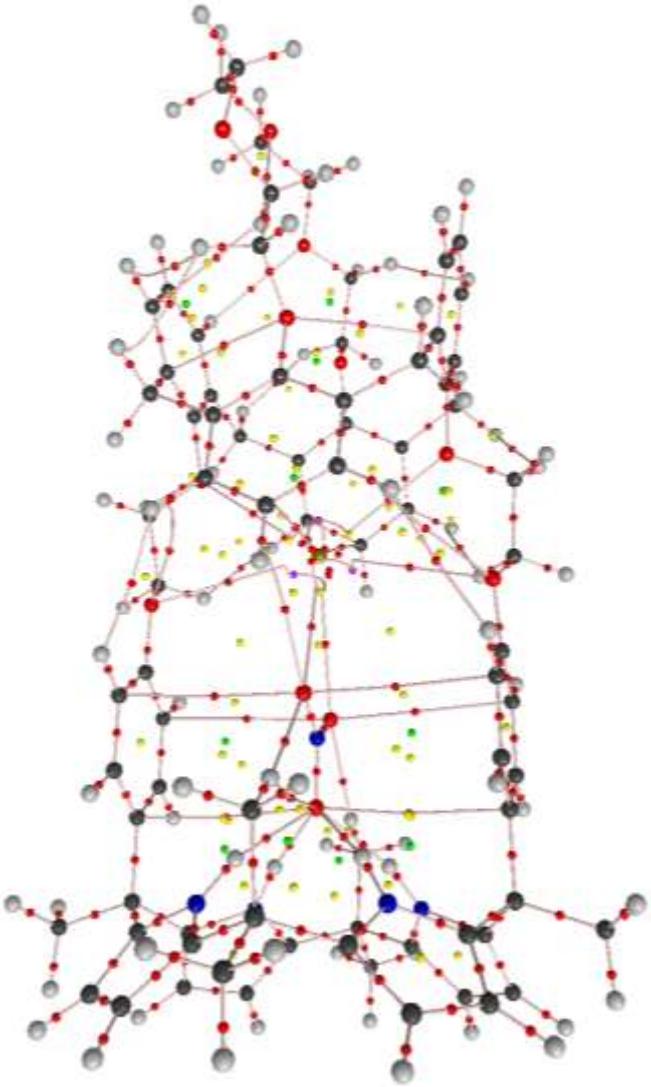
(c) Receptor-$Cs^{+}Br^{-}$ (G/P)



(d) Receptor-$Cs^{+}I^{-}$ (G/P)



(e) Receptor-$Cs^{+}NO_3^{-}$ (G/P)



Optimized Structure coordinates:

1) Receptor-Cs^+ (Crown site) [Energy (Hartree) : -3936.849915740366]

Cs	0.9023330	5.4452106	2.7732953
O	-3.5902218	-0.4255788	1.6608515
O	-2.5351146	2.3487418	1.4530523
O	-0.6120311	6.5625864	0.5262862
O	-0.2575712	8.3102001	2.7644337
O	1.4589080	7.4069516	5.0142076
O	2.0492408	4.5463923	5.5196184
O	1.7785864	2.7155739	3.3583916
O	2.0056910	3.1480606	-1.2116164
O	3.1352131	0.7190334	-2.6460775
N	-0.0057549	-4.9658805	-4.3450789
H	-0.1311678	-4.9073128	-3.3324532
N	-2.7459580	-5.2895972	-2.3230310
H	-2.6016150	-4.3025636	-2.0950949
N	-0.6921592	-5.9853446	0.2684742
H	-0.5931670	-5.2500553	-0.4321969
N	2.1018472	-5.2939553	-1.7099417
H	2.0100666	-4.3028564	-1.4708625
C	1.2304292	-5.0486815	-4.9653914
C	0.9811397	-5.2790939	-6.3188096
H	1.7403005	-5.3845923	-7.1038524
C	-0.4404397	-5.3295036	-6.5000145
H	-0.9690238	-5.4810654	-7.4493747
C	-1.0381843	-5.1275818	-5.2539261
C	-2.4993481	-4.9446515	-4.8519329
C	-2.8544981	-5.7788021	-3.6227575
C	-3.3796012	-7.0669156	-3.5155458
H	-3.5813813	-7.7485229	-4.3518506
C	-3.6255244	-7.3319502	-2.1312309
H	-4.0296045	-8.2625022	-1.7123514
C	-3.2475660	-6.2042342	-1.4021122
C	-3.2225671	-5.9732611	0.1107941
C	-1.9073714	-6.5219921	0.6585261
C	-1.6185526	-7.5246382	1.5849646
H	-2.3541476	-8.1518317	2.1037827
C	-0.1934449	-7.5741815	1.7465302
H	0.3627312	-8.2488371	2.4091427
C	0.3653965	-6.5989597	0.9179131
C	1.8062565	-6.1489577	0.6926890
C	2.1856418	-6.3234493	-0.7778152
C	2.6346763	-7.4480918	-1.4716691
H	2.7880131	-8.4470153	-1.0427887
C	2.8559597	-7.0701955	-2.8337296
H	3.2007036	-7.7279466	-3.6422858
C	2.5384998	-5.7178921	-2.9607275
C	2.5232406	-4.8109493	-4.1932496

C	-3.4066429	-5.3702078	-6.0289999
H	-3.2361479	-6.4298558	-6.3151203
H	-3.2064283	-4.7391738	-6.9216390
H	-4.4757853	-5.2498372	-5.7515060
C	-2.7479479	-3.4346894	-4.5650602
H	-3.8009970	-3.2529846	-4.2535382
H	-2.5461867	-2.8394322	-5.4813894
H	-2.0709483	-3.0374537	-3.7749173
C	-4.4038955	-6.7392058	0.7620008
H	-5.3682953	-6.3645274	0.3586211
H	-4.3993230	-6.5862033	1.8621301
H	-4.3391471	-7.8304727	0.5639659
C	1.9549874	-4.6647774	1.1289813
H	2.9930408	-4.3001740	0.9620138
H	1.7203906	-4.5644600	2.2103657
H	1.2555205	-3.9853012	0.5905277
C	2.7506832	-7.0056327	1.5661599
H	2.6765896	-8.0846437	1.3141313
H	2.4974868	-6.8874729	2.6421799
H	3.8043187	-6.6857606	1.4164637
C	3.7275433	-5.1655964	-5.1062524
H	4.6820037	-5.0278118	-4.5557967
H	3.7421167	-4.5057116	-5.9996897
H	3.6708230	-6.2195868	-5.4530515
C	-3.3600805	-4.4728315	0.4847577
C	-4.1419407	-3.5661230	-0.2626216
H	-4.6974444	-3.9136110	-1.1495183
C	-4.2470264	-2.2046021	0.0890337
H	-4.8466047	-1.5344544	-0.5447058
C	-3.5918236	-1.7273679	1.2434158
C	-2.8702825	-2.6393664	2.0471963
H	-2.3869443	-2.2765599	2.9683467
C	-2.7518035	-3.9782018	1.6634980
H	-2.1651108	-4.6617865	2.2983487
C	-4.0786336	0.5868085	0.7748930
H	-5.1642315	0.4338309	0.5737137
H	-3.5298532	0.5464810	-0.1946467
C	-3.9171235	1.9465714	1.4261057
H	-4.5289889	2.6719884	0.8418833
H	-4.3248001	1.9119565	2.4625078
C	-2.2477345	3.2883140	2.4242123
C	-2.6666605	4.6418007	2.2797629
C	-2.5517196	5.4891968	3.4042830
H	-2.9080494	6.5299881	3.3274217
C	-1.9870084	5.0340822	4.6068801
H	-1.9325673	5.7032518	5.4811981
C	-1.4403970	3.7412930	4.6713322
H	-0.9323185	3.4059209	5.5906436
C	-1.5357069	2.8550375	3.5774205
C	-0.9307161	1.4562083	3.6602800

H	-1.7490658	0.7082160	3.5773280
H	-0.5005411	1.3332074	4.6776976
C	0.1009950	1.1067833	2.5844349
C	1.3659768	1.7432192	2.4518440
C	2.2103302	1.4911210	1.3372305
C	1.8220962	0.4961970	0.4195087
H	2.4683922	0.3014714	-0.4496201
C	0.6209106	-0.2052474	0.5781282
H	0.3296277	-0.9783459	-0.1518465
C	-0.2382324	0.1222787	1.6343529
H	-1.2212196	-0.3642866	1.7171370
C	3.5002292	2.2711972	1.0845602
H	4.0505728	1.7449157	0.2732868
H	4.1543725	2.2359246	1.9825186
C	3.3313434	3.7404093	0.6977904
C	2.5126325	4.1393308	-0.3966228
C	2.2163757	5.5117063	-0.6396966
C	2.9342149	6.4770732	0.1017865
H	2.7544716	7.5463073	-0.1036772
C	3.8620125	6.1037512	1.0884848
H	4.4280260	6.8743787	1.6373133
C	4.0184382	4.7449384	1.4122157
H	4.6968299	4.4491434	2.2306745
C	1.1640739	5.9800303	-1.6493522
H	1.0939456	7.0850351	-1.5548242
H	1.5209158	5.7924219	-2.6866520
C	-0.2293944	5.3664036	-1.5210929
C	-1.0857945	5.6673494	-0.4274347
C	-2.3431346	5.0232441	-0.2647479
C	-2.7737351	4.1601496	-1.2937742
H	-3.7600528	3.6751259	-1.2033634
C	-1.9794472	3.9076956	-2.4208911
H	-2.3436859	3.2371071	-3.2163848
C	-0.7081792	4.4904423	-2.5159534
H	-0.0731519	4.2744106	-3.3911774
C	-3.2265091	5.2012764	0.9711193
H	-3.4492758	6.2762423	1.1406603
H	-4.2110342	4.7351759	0.7460499
C	2.2542764	2.2984477	4.6495324
H	2.9824683	1.4624674	4.5389558
H	1.4104762	1.9449168	5.2852473
C	2.9574024	3.4665234	5.3240195
H	3.3596689	3.1050390	6.3029150
H	3.8272600	3.7998961	4.7040040
C	2.6224301	5.6510337	6.2180438
H	3.5598597	5.9915664	5.7107623
H	2.8926324	5.3495191	7.2600758
C	1.6351395	6.8051798	6.2969015
H	0.6561427	6.4395471	6.6955723
H	2.0361856	7.5563325	7.0210922

C	0.5785737	8.5306945	5.0315830
H	0.9633579	9.3080696	5.7366704
H	-0.4379826	8.2265288	5.3853300
C	0.4779246	9.1562549	3.6487799
H	-0.0331857	10.1453998	3.7478956
H	1.5046970	9.3448331	3.2462556
C	-0.2894421	8.7860892	1.4221173
H	0.7467244	8.8302477	1.0022186
H	-0.7144119	9.8195698	1.3792630
C	-1.1658258	7.8915894	0.5585396
H	-2.2032420	7.8756824	0.9633725
H	-1.1993700	8.3170444	-0.4703622
C	2.6227962	3.0710008	-2.5087978
H	3.7284092	3.1786854	-2.4185762
H	2.2534134	3.8875362	-3.1700556
C	2.2880676	1.7480330	-3.1707312
H	1.2156710	1.5024687	-2.9940511
H	2.4537315	1.8435515	-4.2688222
C	2.9434816	-0.5650659	-3.0739017
C	3.8054710	-1.5460844	-2.5293130
H	4.5933418	-1.2337671	-1.8251077
C	3.6588679	-2.8925834	-2.8860312
H	4.3532827	-3.6300849	-2.4490138
C	2.6479588	-3.3173450	-3.7852040
C	1.8176584	-2.3212641	-4.3353148
H	1.0381218	-2.6014222	-5.0609595
C	1.9531759	-0.9620048	-3.9958246
H	1.2734137	-0.2300886	-4.4554980

2) Receptor-Cs^+ (Glycol site) [Energy (Hartree) : -3936.846636768254]

Cs	-0.2333533	0.0514101	-1.1606845
O	2.6116134	-2.0407404	-0.6471166
O	1.9789405	-0.6849901	-3.1903791
O	-0.8660382	1.0556598	-6.2043362
O	-0.8216167	3.1644607	-8.2637806
O	1.0456859	5.4727783	-7.9722796
O	2.3159454	6.3990674	-5.3331548
O	1.6872258	3.4431603	-3.3937807
O	-2.1520909	2.2763130	-2.0312207
O	-2.5169701	1.5859622	0.7365355
N	1.9973062	-2.5174401	5.6193986
H	1.8224806	-2.0003321	4.7539615
N	-0.2753535	-4.9178382	4.5313414
H	-0.3933291	-3.9045818	4.4775006
N	-2.7913111	-2.8815457	5.1384576
H	-2.5828076	-2.5559941	4.1903731
N	-0.4976649	-0.6799806	6.5885379
H	-0.3549824	-1.4431335	5.9236109
C	2.2131908	-1.9224810	6.8612337
C	2.7030808	-2.9253047	7.6981468

H	2.9694749	-2.8037851	8.7556296
C	2.8150657	-4.1276799	6.9311500
H	3.1628124	-5.1006680	7.3013994
C	2.3923232	-3.8508397	5.6305252
C	2.2585474	-4.7871026	4.4248926
C	0.9507518	-5.5610941	4.5530382
C	0.6822306	-6.9235819	4.6908066
H	1.4299918	-7.7248013	4.7406033
C	-0.7414056	-7.0857659	4.7478409
H	-1.2834340	-8.0347438	4.8444729
C	-1.3206555	-5.8192728	4.6395986
C	-2.7766349	-5.3713618	4.5349867
C	-3.0511805	-4.2055556	5.4809700
C	-3.5657879	-4.1839484	6.7782849
H	-3.8626300	-5.0628412	7.3647343
C	-3.6422187	-2.8200165	7.2022577
H	-3.9935694	-2.4619331	8.1788430
C	-3.1730818	-2.0197283	6.1600126
C	-2.9794674	-0.5017672	6.1011928
C	-1.7331579	-0.1356351	6.8976727
C	-1.5166191	0.7840240	7.9242110
H	-2.2837135	1.4036880	8.4050786
C	-0.1140404	0.7856130	8.2221265
H	0.3892804	1.4097107	8.9712190
C	0.5053675	-0.1316445	7.3696292
C	1.9796400	-0.4365558	7.1141269
C	3.4427100	-5.7923535	4.4376714
H	4.4065694	-5.2465352	4.3587401
H	3.3621030	-6.4915826	3.5782494
H	3.4547784	-6.3912757	5.3730467
C	-3.6997096	-6.5535686	4.9038387
H	-3.4974432	-6.9267435	5.9303049
H	-3.5479064	-7.3982223	4.1978341
H	-4.7646983	-6.2415077	4.8478857
C	-3.0743373	-4.9556753	3.0645646
H	-4.1257186	-4.6075087	2.9543666
H	-2.9180353	-5.8243292	2.3889060
H	-2.3975606	-4.1468893	2.7077812
C	-4.2102826	0.1953625	6.7427645
H	-5.1362848	-0.0798697	6.1953660
H	-4.0940437	1.2995030	6.7012475
H	-4.3300422	-0.1029965	7.8061488
C	2.4484009	0.3902062	5.8784890
H	3.5166968	0.1852087	5.6428326
H	2.3332390	1.4762103	6.0846882
H	1.8391236	0.1708325	4.9725302
C	2.8111975	0.0075112	8.3381176
H	2.4845759	-0.5111252	9.2645248
H	2.7034267	1.1010036	8.5027884
H	3.8878464	-0.2117463	8.1725363

C	2.3101650	-4.0256945	3.0735302
C	3.2036516	-2.9481821	2.8559808
H	3.8709573	-2.6096834	3.6659207
C	3.2871837	-2.3022839	1.6135317
H	3.9883127	-1.4661353	1.4611582
C	2.4916173	-2.7372054	0.5315611
C	1.6287716	-3.8373498	0.7119218
H	1.0091689	-4.2185798	-0.1138716
C	1.5428210	-4.4568249	1.9713308
H	0.8594507	-5.3129920	2.0867808
C	2.2522283	-2.7067038	-1.8636037
H	1.1478406	-2.8532620	-1.9313225
H	2.7298015	-3.7126153	-1.9009685
C	2.7445757	-1.8976701	-3.0461565
H	3.8241033	-1.6550082	-2.9150200
H	2.6426464	-2.5273169	-3.9595024
C	3.7626820	1.5341091	-2.6432945
H	4.5762796	2.2875571	-2.7519802
H	4.2329350	0.6648484	-2.1327923
C	2.4012439	0.0877568	-4.2779004
C	3.3221105	1.1378629	-4.0449813
C	3.8539623	1.8085326	-5.1645554
H	4.6007160	2.6045755	-5.0034358
C	3.4454107	1.4834956	-6.4656967
H	3.8755238	2.0142584	-7.3307147
C	2.4541593	0.5107932	-6.6586603
H	2.0970638	0.2863545	-7.6775624
C	1.9023124	-0.1992466	-5.5730352
C	0.8095811	-1.2354002	-5.8243443
H	1.1809806	-2.2560597	-5.5813648
H	0.6086845	-1.2433964	-6.9181476
C	-0.5005815	-1.0305212	-5.0721553
C	-0.9747726	-2.0217442	-4.1871387
H	-0.3904048	-2.9490384	-4.0589562
C	-2.1860928	-1.8575344	-3.4941620
H	-2.5569835	-2.6521858	-2.8253882
C	-2.9127700	-0.6644549	-3.6456104
H	-3.8496138	-0.5192585	-3.0806985
C	-2.4769223	0.3570087	-4.5173103
C	-1.2913288	0.1341926	-5.2714787
C	-3.2797490	1.6502444	-4.6243717
H	-3.7188587	1.7426052	-5.6420053
H	-4.1486151	1.5609779	-3.9359750
C	-2.5073039	2.9331754	-4.3369820
C	-1.9180853	3.1816100	-3.0727561
C	-1.1013910	4.3145642	-2.8353584
C	-1.0119944	5.2804718	-3.8587184
H	-0.4117406	6.1898331	-3.6879051
C	-1.6492365	5.0936815	-5.0928137
H	-1.5568047	5.8566981	-5.8823978

C	-2.3595277	3.9113693	-5.3394016
H	-2.7966207	3.7357109	-6.3347792
C	-0.3537161	4.5257813	-1.5252569
H	-1.0711293	4.5304754	-0.6754786
H	0.0743990	5.5540835	-1.5487705
C	0.7611047	3.5431795	-1.1531977
C	1.7269433	3.0470336	-2.0775308
C	2.7150579	2.0999630	-1.6823254
C	2.7764952	1.7282328	-0.3212962
H	3.5492259	1.0106053	0.0014005
C	1.8839812	2.2650355	0.6207250
H	1.9624022	1.9807659	1.6831391
C	0.8767058	3.1476712	0.1981276
H	0.1550693	3.5474714	0.9301244
C	-1.5473865	0.9935448	-7.4688350
H	-2.5851299	1.3921295	-7.3798176
H	-1.6189292	-0.0664305	-7.8092640
C	-0.7932733	1.7761953	-8.5275503
H	0.2621848	1.4096357	-8.5872658
H	-1.2802161	1.5476206	-9.5121485
C	-0.2146865	3.9172137	-9.3009494
H	-0.8418531	3.8829389	-10.2297579
H	0.7888482	3.4948584	-9.5608520
C	-0.0344093	5.3660261	-8.8825602
H	0.1677840	5.9771820	-9.8001234
H	-0.9842923	5.7501563	-8.4302954
C	1.3260954	6.8052580	-7.5823419
H	0.4496895	7.2647943	-7.0558980
H	1.5420234	7.4404757	-8.4822680
C	2.5454056	6.8378523	-6.6634152
H	3.3686851	6.2448646	-7.1376492
H	2.8845505	7.8932877	-6.5766069
C	2.1325589	4.9942976	-5.1705827
H	2.8793442	4.4285123	-5.7766969
H	1.1227419	4.6655387	-5.5038853
C	2.2996808	4.7065803	-3.6788211
H	3.3758947	4.6896398	-3.3833894
H	1.8070898	5.5243069	-3.1021361
C	-3.3381651	2.5944121	-1.2763446
H	-4.2264681	2.6268938	-1.9484829
H	-3.2292282	3.5966293	-0.8015913
C	-3.5921830	1.5478480	-0.2090478
H	-4.5567027	1.7933625	0.2906977
H	-3.6819292	0.5307240	-0.6584273
C	-2.6942189	1.0419812	1.9835660
C	-1.7614233	1.4362660	2.9647490
H	-0.9787373	2.1630044	2.6956285
C	-1.8437086	0.9262728	4.2652000
H	-1.1135986	1.2729397	5.0120795
C	-2.8508203	0.0066414	4.6390746

C	-3.7877712	-0.3616749	3.6474868
H	-4.6087951	-1.0555726	3.8953819
C	-3.7189442	0.1369837	2.3314248
H	-4.4662334	-0.1904994	1.5927211

3) Receptor-Cs^+ (Pyrrole site) [Energy (Hartree) : -3936.836604488540]

O	-3.4417343	2.7193191	-0.0134779
O	-2.5364465	1.8429813	-2.7557321
O	-1.1952566	-0.9767063	-6.0818343
O	0.1535918	-0.6552596	-8.7982839
O	2.5806990	1.9460451	-8.1222415
O	4.1505001	2.9910771	-5.8567431
O	1.8605666	2.3626704	-3.8424517
O	1.2544260	-1.7787873	-2.2519885
O	3.5054802	-2.4423118	-0.2627606
N	-2.8182296	-0.8982833	5.1916868
H	-2.4727237	-0.7240161	4.2449818
N	0.0434188	-3.0026016	5.1383032
H	0.0454901	-2.4276164	4.2934107
N	2.1069355	-0.3308691	5.5217408
H	1.8730235	-0.2725056	4.5279199
N	-0.7669096	1.7919125	5.6512869
H	-0.6809793	1.4898210	4.6787880
C	-3.0357788	-2.1641606	5.7241618
C	-3.7815726	-1.9771091	6.8907347
H	-4.1186248	-2.7679140	7.5729357
C	-4.0374554	-0.5743165	7.0327056
H	-4.5964778	-0.0989342	7.8484505
C	-3.4448014	0.0821745	5.9523725
C	-3.3111420	1.5740999	5.6369080
C	-1.9943501	2.0571766	6.2478303
C	-1.7174608	2.7103880	7.4491182
H	-2.4581101	3.0486770	8.1843325
C	-0.2954281	2.8624393	7.5506436
H	0.2458539	3.3428797	8.3752403
C	0.2816271	2.3022589	6.4089595
C	1.7440564	2.1639888	5.9833131
C	2.2526837	0.7706045	6.3575527
C	2.8641745	0.3013964	7.5228301
H	3.1143195	0.9032576	8.4057785
C	3.1139829	-1.1001933	7.3586577
H	3.5824709	-1.7638727	8.0962189
C	2.6517715	-1.4737814	6.0953919
C	2.5760582	-2.8444338	5.4187823
C	1.2115642	-3.4526417	5.7443919
C	0.8300250	-4.4301706	6.6629753
H	1.5020774	-4.9837938	7.3301884
C	-0.5928919	-4.5852286	6.5764586
H	-1.2042123	-5.2826015	7.1625276
C	-1.0655091	-3.7018404	5.6042767

C	-2.4783958	-3.4362514	5.0833702
C	-4.4880579	2.3399003	6.2959835
H	-4.5089010	2.1910181	7.3965009
H	-5.4532742	1.9833929	5.8784386
H	-4.3940426	3.4279873	6.0947822
C	-2.4654467	-3.3078731	3.5370365
H	-1.8161318	-2.4813048	3.1654573
H	-3.4914572	-3.1195751	3.1526446
H	-2.0867899	-4.2458758	3.0771120
C	-3.3872641	-4.6278219	5.4622833
H	-2.9992736	-5.5660725	5.0105471
H	-4.4194396	-4.4536032	5.0895173
H	-3.4408379	-4.7744763	6.5613980
C	3.6892494	-3.7565764	5.9971537
H	3.5893972	-3.8762095	7.0969266
H	4.6871132	-3.3185630	5.7840422
H	3.6366152	-4.7634559	5.5318051
C	2.5883007	3.2242566	6.7272605
H	2.5277671	3.1028201	7.8290140
H	2.2299400	4.2455972	6.4755251
H	3.6560453	3.1381299	6.4318465
C	1.8924362	2.4121444	4.4593526
H	2.9562101	2.3192091	4.1508835
H	1.5418614	3.4338879	4.1989707
H	1.3054819	1.6997318	3.8333493
C	-3.3501431	1.8435471	4.1122487
C	-4.1287112	1.0542761	3.2390189
H	-4.7142247	0.2083859	3.6355574
C	-4.1987178	1.3144700	1.8574149
H	-4.8157603	0.6597529	1.2251152
C	-3.4835443	2.4023256	1.3099599
C	-2.7477648	3.2409868	2.1802801
H	-2.2236285	4.1156521	1.7631891
C	-2.6874347	2.9628668	3.5503563
H	-2.1120792	3.6434513	4.1991434
C	-4.1347605	1.8816259	-0.9466530
H	-5.2330202	1.9557384	-0.7716060
H	-3.8224531	0.8198885	-0.8201378
C	-3.8242618	2.3294458	-2.3627250
H	-4.6227505	1.9295146	-3.0308917
H	-3.8625846	3.4432664	-2.4246151
C	-2.1205350	2.2778906	-4.0040938
C	-2.6310842	1.6799077	-5.1858799
C	-2.2750432	2.2583826	-6.4212788
H	-2.6905500	1.8271140	-7.3477375
C	-1.4023217	3.3540458	-6.4938690
H	-1.1464160	3.7958716	-7.4711152
C	-0.8189214	3.8507874	-5.3187604
H	-0.0936637	4.6804966	-5.3716845
C	-1.1553799	3.3153341	-4.0602919

C	-0.5025469	3.8411807	-2.7900676
H	0.1227778	4.7193297	-3.0656429
H	-1.2853925	4.2290147	-2.1019060
C	0.3171804	2.8179149	-2.0048723
C	1.4287779	2.1190999	-2.5516656
C	2.0831196	1.0954147	-1.8182487
C	1.6599595	0.8289108	-0.5018161
H	2.1669556	0.0316792	0.0660321
C	0.6036492	1.5477792	0.0734276
H	0.2751038	1.3290018	1.1037037
C	-0.0706496	2.5153097	-0.6842395
H	-0.9507254	3.0273526	-0.2644234
C	3.2104775	0.2774607	-2.4354284
H	3.6328211	-0.3665127	-1.6332027
H	4.0263333	0.9535801	-2.7736620
C	2.8139297	-0.5912050	-3.6229228
C	1.8139658	-1.5916624	-3.5036674
C	1.3491577	-2.3058440	-4.6426898
C	2.0422101	-2.1270461	-5.8573327
H	1.7117158	-2.6884449	-6.7477880
C	3.1053261	-1.2194017	-5.9651644
H	3.6369275	-1.1052594	-6.9237589
C	3.4490430	-0.4192254	-4.8670745
H	4.2061242	0.3746657	-4.9742325
C	0.1112022	-3.1985995	-4.6219903
H	0.2632962	-4.0808725	-3.9616098
H	-0.0073882	-3.6208590	-5.6435250
C	-1.1819336	-2.5153459	-4.1833643
C	-1.7604543	-1.4350182	-4.9039364
C	-2.9199498	-0.7688763	-4.4257087
C	-3.5366446	-1.2504498	-3.2540150
H	-4.4540969	-0.7566040	-2.8911918
C	-3.0140037	-2.3499220	-2.5581815
H	-3.5148866	-2.7220285	-1.6488467
C	-1.8369745	-2.9600685	-3.0161230
H	-1.4089863	-3.8091788	-2.4564456
C	-3.5078400	0.4301781	-5.1624874
H	-4.4986153	0.6545189	-4.7069915
H	-3.7179896	0.1543472	-6.2190448
C	2.6439403	3.5462963	-4.0328528
H	3.5888338	3.4957570	-3.4386089
H	2.0817323	4.4452043	-3.6883255
C	2.9749812	3.7188444	-5.5068314
H	2.1026753	3.3862761	-6.1139395
H	3.1442760	4.8087960	-5.7017703
C	4.5058970	3.1100950	-7.2306353
H	5.6185782	3.1012762	-7.2866738
H	4.1557135	4.0886002	-7.6411536
C	3.9974297	1.9652880	-8.1008094
H	4.4214211	2.0910217	-9.1323585

H	4.3898708	0.9987487	-7.6972932
C	2.0213749	0.8257450	-8.7908014
H	2.6897076	-0.0644181	-8.7023787
H	1.8898941	1.0324699	-9.8839216
C	0.6773302	0.4991591	-8.1426386
H	0.8202616	0.3248038	-7.0526599
H	-0.0213687	1.3633774	-8.2582827
C	-1.2074933	-0.9458122	-8.5231611
H	-1.5717920	-1.5624395	-9.3760309
H	-1.8101015	-0.0052110	-8.4974874
C	-1.4659448	-1.7563242	-7.2553317
H	-2.5347245	-2.0811272	-7.2615704
H	-0.8321714	-2.6746693	-7.2769480
C	1.4729982	-3.0288812	-1.5974904
H	1.1171627	-3.8866635	-2.2145567
H	0.8373708	-2.9867492	-0.6889042
C	2.9299184	-3.3270797	-1.2356622
H	3.0146094	-4.3842999	-0.8956478
H	3.5735233	-3.2129483	-2.1330210
C	3.2413158	-2.6111569	1.0655403
C	2.4037834	-3.6079936	1.6118709
H	1.9040862	-4.3527213	0.9757070
C	2.1888101	-3.6581579	3.0009955
H	1.5356667	-4.4538927	3.3949676
C	2.7850330	-2.7365279	3.8875522
C	3.6634174	-1.7781037	3.3247499
H	4.2013734	-1.0712542	3.9778384
C	3.8828682	-1.7064463	1.9435896
H	4.5652644	-0.9505107	1.5233186
Cs	-0.5102944	-0.9413728	8.1088514

Receptor-$Cs^{+}F^{-}.CH_3OH$ (C/P) Energy (Hartree): -4152.624407254656

Cs	17.4741961	12.5498916	9.6164993
O	13.8133769	6.9204049	13.0832159
O	14.4614451	9.6339757	11.9206079
O	16.7525362	13.6055257	12.2583002
O	17.5508870	15.5573606	10.3117954
O	17.9145121	14.6892694	7.5057082
O	18.4712152	11.8709631	6.7530651
O	17.7361531	9.8216274	8.5943620
O	19.5411715	9.9956531	12.9131039
O	20.9986649	10.1727198	15.6606237
N	19.8455402	4.2785925	18.2173797
H	19.0603542	4.8321350	17.8038904
N	17.0534383	2.8593926	17.0707350
H	17.2231062	3.8917709	17.1243478
N	15.2711862	4.9137613	18.9158523
H	16.0118180	5.2581870	18.2646515
N	18.0586017	6.3603566	20.0335834
H	17.8722117	6.1674574	19.0230605

C	20.6612062	4.7267944	19.2422397
C	21.5152150	3.6706713	19.5777337
H	22.2996016	3.6931456	20.3449589
C	21.1978484	2.5695435	18.7219408
H	21.6976674	1.5923943	18.7090556
C	20.1570740	2.9728783	17.8761244
C	19.5125160	2.2497059	16.6922760
C	18.0426514	1.9003611	16.9317128
C	17.4078825	0.6526017	16.9565301
H	17.8986317	-0.3237092	16.8584576
C	16.0038593	0.8824053	17.1076949
H	15.2215501	0.1146455	17.1538026
C	15.8065464	2.2659064	17.1751344
C	14.5166016	3.0696321	17.3349327
C	14.4890757	3.7980540	18.6797793
C	13.6833176	3.6149230	19.8079540
H	12.9299947	2.8284883	19.9440521
C	13.9941139	4.6626756	20.7344745
H	13.5240956	4.8262713	21.7125770
C	14.9818496	5.4653523	20.1510621
C	15.6093499	6.7765640	20.6238489
C	17.0858394	6.6210035	20.9835994
C	17.7419838	6.7794983	22.2093772
H	17.2658754	7.0080150	23.1713633
C	19.1443301	6.6152281	21.9746154
H	19.9424707	6.6928447	22.7238512
C	19.3165499	6.3574550	20.6109620
C	20.5894517	6.1516639	19.7924949
C	20.2910698	0.9402525	16.4349328
H	20.2388477	0.2510713	17.3048924
H	21.3610321	1.1617347	16.2335294
H	19.8742637	0.4108913	15.5513364
C	19.6374918	3.1370103	15.4174842
H	19.1164867	4.1137496	15.5084025
H	19.2032458	2.6057172	14.5411518
H	20.7102452	3.3475164	15.2062646
C	13.3164973	2.0893551	17.2750996
H	13.3716075	1.3307933	18.0856618
H	13.3042955	1.5579946	16.2999170
H	12.3615202	2.6455695	17.3824365
C	15.4690494	7.8448485	19.4983647
H	16.0121485	7.5496167	18.5745874
H	15.8848835	8.8187404	19.8406901
H	14.3976750	7.9877076	19.2336649
C	14.8419509	7.2767040	21.8661581
H	14.9107626	6.5579131	22.7106255
H	13.7670887	7.4195890	21.6231813
H	15.2549092	8.2496822	22.2095482
C	21.8133328	6.3864959	20.7163545
H	21.8151769	5.6813522	21.5752735

H	21.7969373	7.4224249	21.1165549
H	22.7556520	6.2467065	20.1459059
C	14.3329585	4.1065884	16.1911335
C	14.9594457	3.9720804	14.9333355
H	15.6384007	3.1239692	14.7495084
C	14.7659025	4.9133034	13.9136469
H	15.2886256	4.8085172	12.9498510
C	13.9263657	6.0293419	14.1190806
C	13.2612391	6.1627922	15.3574569
H	12.5894302	7.0100533	15.5580867
C	13.4715218	5.2082897	16.3679341
H	12.9524675	5.3410281	17.3313412
C	13.1271970	8.1466354	13.3303248
H	13.5842173	8.6723053	14.2000082
H	12.0545387	7.9466436	13.5646729
C	13.1631857	9.0402368	12.1059458
H	12.8665292	8.4551802	11.2032923
H	12.4004050	9.8412142	12.2524039
C	14.4612644	10.5790327	10.9113802
C	14.6869691	10.1661361	9.5680847
C	14.4714042	11.1096714	8.5406576
H	14.5963682	10.7936389	7.4909794
C	14.0978192	12.4326432	8.8328077
H	13.9118330	13.1501442	8.0162756
C	14.0195893	12.8502315	10.1717752
H	13.7891476	13.9035837	10.4055234
C	14.2193205	11.9436262	11.2362806
C	14.1507685	12.4468894	12.6793052
H	13.9761837	13.5441341	12.6377440
H	13.2574427	12.0128159	13.1815248
C	15.3611475	12.1410554	13.5583458
C	16.6452602	12.6953063	13.3074090
C	17.7906444	12.2814073	14.0401015
C	17.5909137	11.3970439	15.1204080
H	18.4720634	11.0559620	15.6875642
C	16.3150438	10.9249629	15.4561534
H	16.1845992	10.2444881	16.3124734
C	15.2168117	11.2750446	14.6599358
H	14.2179442	10.8689589	14.8903012
C	19.2213925	12.7233456	13.7232032
H	19.8643786	12.3084017	14.5293444
H	19.3135866	13.8285856	13.8025426
C	19.8006867	12.3129092	12.3702710
C	19.8966580	10.9454301	11.9815024
C	20.3099648	10.5790631	10.6638669
C	20.8222898	11.6011651	9.8325662
H	21.1794486	11.3356716	8.8232407
C	20.8673940	12.9403327	10.2536559
H	21.2915249	13.7148450	9.5939160
C	20.3170304	13.2931023	11.4969321

H	20.2931000	14.3519224	11.8045817
C	20.2209438	9.1545296	10.1027647
H	20.5080729	9.2122510	9.0315545
H	20.9968860	8.5093127	10.5728606
C	18.8764845	8.4483637	10.2717364
C	17.7008498	8.8230250	9.5647695
C	16.4319214	8.2766521	9.8934901
C	16.3715078	7.2813831	10.8897554
H	15.3892476	6.8805753	11.1846440
C	17.5296372	6.8301325	11.5365287
H	17.4705434	6.0817753	12.3440960
C	18.7640400	7.4148097	11.2233460
H	19.6677298	7.0877340	11.7626098
C	15.1444740	8.7490076	9.2197478
H	14.3445722	8.0220912	9.4838698
H	15.2528535	8.6983388	8.1147735
C	16.9332548	14.9946956	12.5854058
H	17.9741330	15.1845072	12.9342326
H	16.2333138	15.2897131	13.4006218
C	16.6360400	15.8507812	11.3639298
H	15.5848103	15.6792623	11.0215637
H	16.7206401	16.9225442	11.6714324
C	17.3687643	16.3782578	9.1585648
H	17.5837641	17.4463811	9.4081554
H	16.3099961	16.3203734	8.8012526
C	18.3092900	15.9515725	8.0420078
H	18.2770897	16.7348375	7.2447853
H	19.3589021	15.9028219	8.4262089
C	18.7229339	14.2607303	6.4101195
H	19.7892303	14.1488323	6.7295969
H	18.6931203	15.0217543	5.5916811
C	18.2102400	12.9438984	5.8478989
H	17.1130971	13.0249165	5.6448430
H	18.7220415	12.7568504	4.8718394
C	17.9169576	10.6292007	6.3276111
H	18.3107224	10.3454665	5.3200813
H	16.8044218	10.7122016	6.2438542
C	18.2844270	9.5185196	7.3004552
H	19.3926975	9.4146412	7.3548358
H	17.8632937	8.5603665	6.9188662
C	20.6081978	9.1721699	13.4182248
H	21.2195124	8.7621080	12.5832758
H	20.1059820	8.3237043	13.9278076
C	21.5578600	9.9003437	14.3717775
H	22.5017156	9.3179391	14.4701873
H	21.8323774	10.8925437	13.9546150
C	20.9338113	9.1607932	16.5882963
C	20.2868871	9.4717302	17.8054130
H	19.8797577	10.4858751	17.9482624
C	20.1617301	8.5029867	18.8095039

H	19.6448754	8.7696571	19.7461428
C	20.6750957	7.1957927	18.6457517
C	21.3397984	6.9120992	17.4382260
H	21.7649466	5.9093884	17.2729178
C	21.4682437	7.8673863	16.4141053
H	21.9773948	7.5733568	15.4847532
F	17.5215790	5.5145926	17.4612292
O	17.8477254	6.3464995	14.9656935
C	17.3923438	7.6797517	15.0194828
H	17.5515221	8.1556579	14.0276743
H	17.9399716	8.2910302	15.7835625
H	16.2966992	7.7546023	15.2502461
H	17.7073360	5.9745885	15.8855576

Receptor-$Cs^{+}Cl^{-}.H_2O$ (C/P) Energy (Hartree): -4473.660432691813

Cs	0.9489870	5.5030539	2.8182374
Cl	-0.3474365	-3.2004411	-1.4586870
O	-3.5552452	-0.4130089	1.7706458
O	-2.4297270	2.3633067	1.5124284
O	-0.5646468	6.6085317	0.5683789
O	-0.2408878	8.3663966	2.7977611
O	1.4641103	7.4841535	5.0648048
O	2.0786604	4.6297211	5.5767449
O	1.8511611	2.7872445	3.4131257
O	2.0787529	3.2132818	-1.1677202
O	3.1858252	0.8041199	-2.6318583
N	0.0058740	-4.7178498	-4.2937973
H	-0.1205014	-4.1455346	-3.4338849
N	-2.6920004	-5.2981051	-2.3134455
H	-2.0237535	-4.5481017	-2.0444239
N	-0.6733423	-5.9097152	0.2860450
H	-0.5794362	-4.9836817	-0.1781372
N	2.0511550	-5.3472595	-1.7013158
H	1.3958183	-4.5506428	-1.5752980
C	1.2420234	-5.0653915	-4.8167357
C	0.9969272	-5.7832964	-5.9916135
H	1.7566356	-6.2124189	-6.6567040
C	-0.4199324	-5.8547775	-6.1706154
H	-0.9439507	-6.3394665	-7.0037275
C	-1.0212581	-5.1774133	-5.1035661
C	-2.4996275	-4.8822511	-4.8386708
C	-3.0370102	-5.6281413	-3.6148533
C	-3.9774421	-6.6614167	-3.5311770
H	-4.4690524	-7.1553367	-4.3785908
C	-4.2019438	-6.9387350	-2.1457644
H	-4.8913470	-7.6880489	-1.7368162
C	-3.3936685	-6.0729624	-1.4032983
C	-3.2267172	-5.9300915	0.1109017
C	-1.8864845	-6.5255544	0.5470048

C	-1.6003330	-7.7170689	1.2204163
H	-2.3351209	-8.4493579	1.5779749
C	-0.1794982	-7.8022416	1.3670700
H	0.3742447	-8.6094616	1.8628419
C	0.3801010	-6.6600801	0.7830966
C	1.8381706	-6.2018847	0.7052269
C	2.3845846	-6.2689172	-0.7228367
C	3.3020345	-7.1542073	-1.3011900
H	3.7808964	-8.0044995	-0.7992115
C	3.5211511	-6.7364074	-2.6524480
H	4.1950053	-7.2096270	-3.3778952
C	2.7327474	-5.6037554	-2.8781548
C	2.5673406	-4.7344526	-4.1280419
C	-3.3128189	-5.3274451	-6.0754692
H	-3.2081965	-6.4159253	-6.2707117
H	-2.9675624	-4.7815274	-6.9795859
H	-4.3914793	-5.1074496	-5.9249976
C	-2.7136755	-3.3516409	-4.6574391
H	-3.7995998	-3.1314023	-4.5493929
H	-2.3337561	-2.8059232	-5.5503516
H	-2.2062467	-2.9326983	-3.7621737
C	-4.3671438	-6.7153913	0.8114215
H	-5.3540824	-6.3046739	0.5104447
H	-4.2695528	-6.6266085	1.9141567
H	-4.3426523	-7.7937758	0.5456717
C	1.9622359	-4.7502910	1.2514206
H	3.0248923	-4.4205593	1.2260958
H	1.6043227	-4.7074344	2.3043654
H	1.3661561	-4.0202849	0.6616282
C	2.6923937	-7.1257109	1.6020023
H	2.6445616	-8.1849849	1.2711013
H	2.3350060	-7.0793305	2.6533241
H	3.7567102	-6.8067650	1.5782095
C	3.7233576	-5.0595851	-5.1114438
H	4.7025182	-4.8355656	-4.6379613
H	3.6265476	-4.4435944	-6.0305924
H	3.7183959	-6.1302677	-5.4074983
C	-3.3513470	-4.4482185	0.5497216
C	-4.1609188	-3.5387394	-0.1576771
H	-4.7124184	-3.8791993	-1.0493544
C	-4.2787947	-2.1895834	0.2298438
H	-4.9319364	-1.5202574	-0.3507938
C	-3.5713214	-1.7184826	1.3584709
C	-2.8209623	-2.6377048	2.1237158
H	-2.2962604	-2.2819533	3.0248564
C	-2.7174229	-3.9744774	1.7204581
H	-2.1030838	-4.6634524	2.3226885
C	-3.9679576	0.5903716	0.8306053
H	-5.0490500	0.4660183	0.5870932
H	-3.3718651	0.4884495	-0.1066863

C	-3.8109984	1.9671805	1.4441255
H	-4.3931706	2.6774007	0.8128823
H	-4.2597526	1.9727203	2.4643511
C	-2.1637034	3.3100032	2.4796597
C	-2.5958765	4.6593182	2.3303431
C	-2.4946847	5.5099327	3.4540905
H	-2.8597698	6.5473911	3.3727983
C	-1.9305422	5.0637303	4.6603623
H	-1.8855771	5.7360339	5.5328523
C	-1.3728106	3.7758438	4.7306769
H	-0.8660850	3.4471840	5.6531813
C	-1.4545727	2.8863660	3.6386997
C	-0.8429924	1.4911642	3.7258105
H	-1.6583527	0.7404953	3.6358029
H	-0.4199062	1.3700833	4.7468367
C	0.1944179	1.1453265	2.6539649
C	1.4483686	1.8012627	2.5124137
C	2.2915673	1.5534371	1.3962077
C	1.9142269	0.5445752	0.4883119
H	2.5567768	0.3539638	-0.3849530
C	0.7288298	-0.1813978	0.6567826
H	0.4504648	-0.9740374	-0.0569195
C	-0.1292262	0.1448139	1.7145971
H	-1.1027476	-0.3610933	1.8018117
C	3.5723394	2.3461478	1.1339756
H	4.1201766	1.8232674	0.3187237
H	4.2337424	2.3172867	2.0272026
C	3.3933204	3.8136264	0.7463793
C	2.5776826	4.2074485	-0.3527484
C	2.2750957	5.5790816	-0.5957365
C	2.9833070	6.5486163	0.1499272
H	2.7971736	7.6168534	-0.0554031
C	3.9075372	6.1807813	1.1418462
H	4.4651784	6.9544439	1.6952780
C	4.0698604	4.8225252	1.4649306
H	4.7448365	4.5298927	2.2874218
C	1.2205859	6.0433651	-1.6052424
H	1.1403700	7.1472043	-1.5055553
H	1.5792886	5.8637318	-2.6433665
C	-0.1660640	5.4141994	-1.4781108
C	-1.0251879	5.7046723	-0.3843322
C	-2.2716905	5.0414594	-0.2168884
C	-2.6881380	4.1654678	-1.2407991
H	-3.6643449	3.6615879	-1.1466185
C	-1.8909469	3.9199050	-2.3669659
H	-2.2408777	3.2314636	-3.1531296
C	-0.6315505	4.5261914	-2.4684370
H	0.0061668	4.3156551	-3.3428559
C	-3.1561437	5.2141295	1.0190993
H	-3.3839029	6.2882163	1.1878827

H	-4.1383061	4.7432168	0.7935850
C	2.3210814	2.3830900	4.7085098
H	3.0623056	1.5567551	4.6089612
H	1.4778300	2.0199046	5.3398930
C	3.0028410	3.5621924	5.3866315
H	3.4041035	3.2075861	6.3684530
H	3.8716643	3.9079095	4.7718897
C	2.6305671	5.7400486	6.2824921
H	3.5704391	6.0920713	5.7875802
H	2.8912340	5.4411366	7.3278190
C	1.6295248	6.8832201	6.3491789
H	0.6491396	6.5064895	6.7338954
H	2.0124111	7.6379713	7.0795579
C	0.5712397	8.5979502	5.0717970
H	0.9395872	9.3803356	5.7802443
H	-0.4456458	8.2826319	5.4147587
C	0.4783931	9.2205593	3.6871823
H	-0.0421340	10.2055676	3.7793270
H	1.5075503	9.4175725	3.2947522
C	-0.2605328	8.8374401	1.4536498
H	0.7800798	8.8850251	1.0452404
H	-0.6897620	9.8688043	1.4022769
C	-1.1224764	7.9351849	0.5834806
H	-2.1659518	7.9186152	0.9731207
H	-1.1425302	8.3546479	-0.4484511
C	2.6796908	3.1515618	-2.4728274
H	3.7863284	3.2592234	-2.3929215
H	2.3037007	3.9760680	-3.1202515
C	2.3429040	1.8354088	-3.1492238
H	1.2694442	1.5867951	-2.9804820
H	2.5123381	1.9489948	-4.2458260
C	2.9968049	-0.4810209	-3.0688073
C	3.7978421	-1.4707749	-2.4547772
H	4.5352618	-1.1647498	-1.6949556
C	3.6379927	-2.8172829	-2.7961826
H	4.2625501	-3.5719058	-2.2897234
C	2.6870070	-3.2328142	-3.7582393
C	1.9316350	-2.2293416	-4.3920117
H	1.1932361	-2.5046556	-5.1616825
C	2.0706504	-0.8676345	-4.0582350
H	1.4362569	-0.1267537	-4.5667468
O	-2.3936853	-0.9003164	-2.0343516
H	-2.9989333	-1.4625114	-1.4974373
H	-1.5342103	-1.3852770	-1.9097026

Receptor-$Cs^{+}NO_3^{-}.C_2H_5OH$ (G/P) Energy (Hartree):-4372.377550396943

Cs	-0.2102166	0.0128714	-1.0769384
O	-2.7403177	-1.7715319	-0.3016205
H	-4.0577869	-2.8768412	-1.3986407
H	-4.1108307	-3.2215739	0.3557579

H	-1.8361859	-4.3510005	0.2073161
C	-2.4712482	-4.1992217	-0.6928269
H	-3.0454164	-5.1364987	-0.8704664
H	-1.7978591	-4.0351244	-1.5637928
C	-3.4195298	-3.0156965	-0.4985350
O	2.7172388	-2.0479575	-0.8381778
O	2.0236487	-0.6333993	-3.3092479
O	-0.6972969	1.3324346	-6.3020587
O	-0.5829438	3.5207197	-8.2717035
O	1.3294136	5.7634695	-7.8362078
O	2.5678610	6.5228273	-5.1275103
O	1.8203767	3.5085705	-3.3243914
O	-2.0484945	2.3994666	-2.0540818
O	-2.5856516	2.0680078	0.8329348
N	2.1529958	-2.2997516	5.4724074
H	1.4765534	-1.9905589	4.7565334
N	-0.0383266	-4.6423641	4.4327707
H	-0.1440897	-3.7047855	4.0103674
N	-2.5651458	-2.6228275	5.2758676
H	-1.8411632	-2.3436921	4.5939854
N	-0.3695353	-0.2701089	6.2810415
H	-0.2540846	-0.5845394	5.3043611
C	2.5883429	-1.5353261	6.5426426
C	3.5258569	-2.3108936	7.2323494
H	4.0762412	-2.0068628	8.1315687
C	3.6586609	-3.5574421	6.5406263
H	4.3228305	-4.3857775	6.8169948
C	2.7981972	-3.5254595	5.4400922
C	2.5206601	-4.5655030	4.3537382
C	1.1868701	-5.2559489	4.6433300
C	0.9209907	-6.5040455	5.2137826
H	1.6678947	-7.2505663	5.5111840
C	-0.4981661	-6.6312028	5.3390679
H	-1.0376703	-7.5002293	5.7355945
C	-1.0813146	-5.4609896	4.8412155
C	-2.5548143	-5.1067714	4.6352777
C	-3.0146469	-3.9184004	5.4816696
C	-3.9949320	-3.8463665	6.4778962
H	-4.5695278	-4.6915012	6.8769274
C	-4.1342380	-2.4752529	6.8599552
H	-4.8240350	-2.0784146	7.6157658
C	-3.2352886	-1.7269401	6.0944356
C	-2.9174994	-0.2311806	6.1171819
C	-1.5995859	-0.0071970	6.8609379
C	-1.3475826	0.4335217	8.1626675
H	-2.1026018	0.7279074	8.9024320
C	0.0717216	0.4399423	8.3515769
H	0.6036251	0.7492730	9.2598028
C	0.6642400	0.0055686	7.1613610
C	2.1366194	-0.0912357	6.7615617

C	3.6492077	-5.6299318	4.3843494
H	4.6307288	-5.1515866	4.1805646
H	3.4647667	-6.4043408	3.6097117
H	3.7080424	-6.1342310	5.3725674
C	-3.4128781	-6.3356777	5.0085917
H	-3.2885380	-6.6183463	6.0759764
H	-3.1258999	-7.2087371	4.3843925
H	-4.4886723	-6.1215399	4.8313792
C	-2.8007116	-4.7877938	3.1317777
H	-3.8772284	-4.5631325	2.9592017
H	-2.5183194	-5.6629726	2.5052960
H	-2.2080551	-3.9152403	2.7815569
C	-4.0501545	0.5084659	6.8770049
H	-5.0205827	0.3535177	6.3596249
H	-3.8367950	1.5977762	6.9119816
H	-4.1495043	0.1404608	7.9205099
C	2.3733874	0.7280745	5.4580526
H	3.4483575	0.6902162	5.1727681
H	2.0870655	1.7915447	5.6180189
H	1.7820939	0.3471098	4.5965265
C	2.9960342	0.5302221	7.8838741
H	2.8732884	-0.0131284	8.8451630
H	2.7070948	1.5904363	8.0483464
H	4.0715188	0.5001350	7.6063765
C	2.5431110	-3.9094440	2.9476270
C	3.3498458	-2.7764746	2.6877310
H	3.9487682	-2.3336849	3.4993861
C	3.4034449	-2.1894844	1.4187893
H	4.0242676	-1.2976238	1.2374748
C	2.6537550	-2.7305038	0.3532345
C	1.8874803	-3.8929518	0.5721283
H	1.3006545	-4.3499952	-0.2390670
C	1.8385944	-4.4626343	1.8595236
H	1.2168941	-5.3597426	2.0129884
C	2.2888967	-2.6972396	-2.0353036
H	1.1796367	-2.8293203	-2.0461512
H	2.7489444	-3.7098700	-2.1115914
C	2.7412465	-1.8805252	-3.2305136
H	3.8354290	-1.6842265	-3.1525202
H	2.5669053	-2.4880580	-4.1482018
C	3.8421345	1.5150107	-2.6036231
H	4.6942232	2.2314071	-2.6563034
H	4.2532153	0.6013073	-2.1205578
C	2.4927163	0.1835195	-4.3446328
C	3.4284434	1.2005928	-4.0330186
C	4.0094858	1.9148623	-5.1006571
H	4.7669561	2.6849437	-4.8750380
C	3.6374561	1.6668306	-6.4288284
H	4.1050360	2.2315937	-7.2520528
C	2.6342607	0.7266811	-6.7003043

H	2.3041560	0.5610165	-7.7397117
C	2.0334624	-0.0253220	-5.6701949
C	0.9267349	-1.0163426	-6.0170049
H	1.2672331	-2.0596292	-5.8309103
H	0.7570504	-0.9493595	-7.1140238
C	-0.3944682	-0.8237923	-5.2840878
C	-0.9058091	-1.8523618	-4.4669220
H	-0.3452933	-2.7995367	-4.3838346
C	-2.1208836	-1.6961741	-3.7826635
H	-2.5231040	-2.5187310	-3.1734032
C	-2.8134878	-0.4779722	-3.8672376
H	-3.7480446	-0.3388995	-3.2979477
C	-2.3433046	0.5772702	-4.6759884
C	-1.1536112	0.3683807	-5.4263562
C	-3.1212307	1.8878007	-4.7267666
H	-3.5348457	2.0438307	-5.7475724
H	-4.0078963	1.7742088	-4.0652529
C	-2.3355892	3.1398429	-4.3550460
C	-1.7724977	3.3247577	-3.0669433
C	-0.9408560	4.4328892	-2.7706691
C	-0.8086143	5.4377360	-3.7518207
H	-0.1956467	6.3269907	-3.5303633
C	-1.4194353	5.3121419	-5.0065722
H	-1.2937002	6.1019167	-5.7644921
C	-2.1438836	4.1531415	-5.3139636
H	-2.5579046	4.0221749	-6.3262932
C	-0.2209089	4.5734479	-1.4380933
H	-0.9577791	4.5424281	-0.6056312
H	0.2204855	5.5960881	-1.4032186
C	0.8719086	3.5571352	-1.0900173
C	1.8349888	3.0676142	-2.0199601
C	2.7972052	2.0878964	-1.6429070
C	2.8403718	1.6820269	-0.2913515
H	3.5912219	0.9357286	0.0164040
C	1.9504211	2.2082326	0.6578306
H	1.9962215	1.8749648	1.7064047
C	0.9646159	3.1193921	0.2493102
H	0.2336744	3.4984064	0.9828472
C	-1.3418048	1.3242465	-7.5854801
H	-2.3802924	1.7250611	-7.5100819
H	-1.4090998	0.2790762	-7.9708106
C	-0.5538361	2.1437694	-8.5903350
H	0.5012765	1.7742497	-8.6328046
H	-1.0120717	1.9580283	-9.5975750
C	0.0543525	4.3113728	-9.2609403
H	-0.5599415	4.3380604	-10.1984882
H	1.0529330	3.8819126	-9.5281925
C	0.2606708	5.7319021	-8.7649889
H	0.4901475	6.3859282	-9.6457818
H	-0.6869243	6.1132198	-8.3053921

C	1.6383445	7.0654938	-7.3730659
H	0.7649589	7.5223653	-6.8393875
H	1.8895130	7.7397723	-8.2348013
C	2.8387118	7.0154438	-6.4303745
H	3.6526730	6.4196630	-6.9172471
H	3.2085321	8.0541733	-6.2868980
C	2.3389765	5.1179413	-5.0310356
H	3.0771799	4.5571093	-5.6516682
H	1.3247585	4.8356088	-5.3921570
C	2.4739958	4.7614252	-3.5510590
H	3.5455578	4.7016363	-3.2425238
H	1.9981285	5.5708255	-2.9485157
C	-3.2887236	2.6902349	-1.3762298
H	-4.1456173	2.5790263	-2.0802403
H	-3.2812384	3.7434525	-1.0116507
C	-3.5160199	1.7501674	-0.2087524
H	-4.5595030	1.9031512	0.1540377
H	-3.4133764	0.6829935	-0.5193001
C	-2.7548308	1.4983315	2.0694528
C	-2.0067038	2.0624292	3.1254798
H	-1.3714559	2.9390957	2.9214903
C	-2.0610800	1.5030850	4.4068687
H	-1.4621686	1.9623003	5.2095043
C	-2.8515822	0.3635228	4.6856556
C	-3.6322650	-0.1525475	3.6323703
H	-4.2847308	-1.0222863	3.8136286
C	-3.5962575	0.3983251	2.3364606
H	-4.1974701	-0.0624821	1.5394279
O	-0.1825329	-1.7873036	3.7749854
O	-0.8923903	-2.1071561	1.7328654
O	0.3313991	-0.3523718	2.1980972
N	-0.2459565	-1.3933985	2.5413435
H	-2.1940539	-1.8460631	0.5256248