

Supplementary Information

Density Functional Theoretical Investigation of Remarkably High Selectivity of Cs⁺ Ion over Na⁺ Ion towards Macrocyclic Hybrid Calix-Bis-crown Ether

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TABLE-S1 (Energies:B3LYP-TZVP)

System	E(hartree)	H (kcal/mol)	S (kj/mol)	G(kcal/mol)
Gas phase				
H ₂ O	-76.42294987	-47941.29261	0.19525	-47955.21935
(H ₂ O) ₆	-458.622643	-287690.1688	0.48292	-287724.6144
Na	-162.0530537	-101688.3486	0.1478	-101698.8909
Cs	-19.97457657	-12532.7545	0.1697	-12544.85882
Na-(H ₂ O) _{6A}	-620.7688983	-389435.9365	0.55955	-389475.848
Na-(H ₂ O) _{6B}	-620.7764264	-389441.0815	0.6251	-389485.6685
Cs-(H ₂ O) _{6A}	-478.6258241	-300242.5869	0.54405	-300281.3928
Cs-(H ₂ O) _{6B}	-478.63407	-300246.3523	0.64795	-300292.5691
18-crown-6	-922.7647273	-578809.0541	0.62724	-578853.7938
18-crown-6-Na	-1084.963109	-680586.5009	0.66394	-680633.8583
18-crown-6-Cs	-942.8209061	-591391.7625	0.69062	-591441.0228
Cal-biscrown6	-2767.031382	-1735685.905	1.30514	-1735778.998
Cal-biscrown6-Na	-2929.222436	-1837459.426	1.33524	-1837554.666
Cal-biscrown6-Cs	-2787.101499	-1748276.688	1.3707	-1748374.457
NO ₃ ⁻	-280.3476596	-175909.8608	0.26169	-175928.5266
NO ₃ ⁻ -(H ₂ O) ₆	-739.0141498	-463625.5508	0.61801	-463669.6321
18-crown-6-Na NO ₃	-1365.45253	-856584.7001	0.77163	-856639.7388
18-crown-6-Cs NO ₃	-1223.282919	-767372.7254	0.84754	-767433.1785
Cal-biscrown6-Na NO ₃	-3209.698825	-2013448.893	1.40496	-2013549.105
Cal-biscrown6-Cs NO ₃	-3067.566904	-1924260.147	1.45289	-1924363.779
Solvent phase(1,2-Dichloroethane)				
H ₂ O	-76.43639285	-47949.72821	0.19525	-47963.65495
(H ₂ O) ₆	-458.6555431	-287710.8139	0.48292	-287745.2595
Na	-162.1976135	-101779.0613	0.1478	-101789.6036
Cs	-20.10407048	-12614.01316	0.1697	-12626.11748
Na-(H ₂ O) _{6A}	-620.8532085	-389488.8419	0.55955	-389528.7534
Na-(H ₂ O) _{6B}	-620.8654679	-389496.9559	0.6251	-389541.5428
Cs-(H ₂ O) _{6A}	-478.7184352	-300300.7013	0.54405	-300339.5072
Cs-(H ₂ O) _{6B}	-478.7290466	-300305.951	0.64795	-300352.1678
18-crown-6	-922.7948119	-578827.9326	0.62724	-578872.6722
18-crown-6-Na	-1085.020902	-680622.7662	0.66394	-680670.1235
18-crown-6-Cs	-942.8854483	-591432.2633	0.69062	-591481.5237
Cal-biscrown6	-2767.060689	-1735704.296	1.30514	-1735797.388
Cal-biscrown6-Na	-2929.285832	-1837499.207	1.33524	-1837594.447
Cal-biscrown6-Cs	-2787.158634	-1748312.54	1.3707	-1748410.309
NO ₃ ⁻	-280.4561002	-175977.9084	0.26169	-175996.5741
NO ₃ ⁻ -(H ₂ O) ₆	-739.1020973	-463680.7387	0.61801	-463724.82
18-crown-6-Na NO ₃	-1365.484592	-856604.8197	0.77163	-856659.8584
18-crown-6-Cs NO ₃	-1223.338353	-767407.5106	0.84754	-767467.9637
Cal-biscrown6-Na NO ₃	-3209.735531	-2013471.926	1.40496	-2013572.139
Cal-biscrown6-Cs NO ₃	-3067.606785	-1924285.173	1.45289	-1924388.804

Coordinates of Optimized complexes and free ligands at BP-TZVP level of theory.

18crown-6

C	-2.9313945	1.2627127	0.1911309
C	-2.6205598	2.6199390	-0.4310377
O	-1.2768180	2.8006318	-0.8715091
C	-0.3821700	3.1796828	0.1689666
C	0.9572874	3.5799467	-0.4402471
O	1.7880530	2.5021034	-0.8631154
C	2.5349250	1.9070533	0.1924709
C	3.5726186	0.9597393	-0.4001789
O	3.0707435	-0.2948672	-0.8534784
C	2.9324034	-1.2627446	0.1812997
C	2.6192957	-2.6198042	-0.4400663
O	1.2740213	-2.8001559	-0.8760175
C	0.3829993	-3.1801435	0.1672221
C	-0.9585197	-3.5798442	-0.4377493
O	-1.7903584	-2.5016166	-0.8575401
C	-2.5344960	-1.9073993	0.2004417
C	-3.5736958	-0.9596274	-0.3887985
O	-3.0728987	0.2949559	-0.8433183
H	-2.1416059	0.9790826	0.9143600
H	-2.8904276	3.4119332	0.2970944
H	-4.3720340	-0.7990630	0.3643570
H	-1.8785345	-1.3677014	0.9120137
H	-1.4998864	-4.2134226	0.2947464
H	0.2462813	-2.3669736	0.9075655
H	2.8914680	-3.4119992	0.2869792
H	2.1449737	-0.9790397	0.9070628
H	4.3732786	0.7991532	0.3505007
H	1.8807634	1.3667980	0.9052499
H	-0.2429203	2.3658597	0.9080833
H	1.5008819	4.2134085	0.2906892
H	-3.2530347	2.7395098	-1.3227753
H	-0.7905625	4.0558440	0.7173652
H	0.7582844	4.1820902	-1.3388825
H	3.0696018	2.6942401	0.7669372
H	4.0161919	1.4474706	-1.2804612
H	3.8857386	-1.3491278	0.7461895
H	3.2487456	-2.7392627	-1.3339539
H	0.7933498	-4.0567807	0.7133618
H	-0.7626283	-4.1817382	-1.3372360
H	-3.0677195	-2.6950467	0.7756175
H	-4.0201028	-1.4469970	-1.2678570
H	-3.8829087	1.3489229	0.7591192

18crown-6-Na

C	-3.0932204	1.8949190	0.3893234
C	-3.4224490	0.4702758	0.7685603
O	-2.7184563	-0.4050736	-0.1189043
O	-1.6654184	2.0357910	0.3395090

C	-1.2449924	3.4102508	0.2756475
C	0.0148196	3.4949087	-0.5554443
O	0.9681591	2.5870258	0.0054152
C	2.2461571	2.6579738	-0.6353201
C	3.1967404	1.7708237	0.1355820
O	2.6079581	0.4651146	0.2523164
C	3.5891008	-0.5754924	0.3661249
C	2.8941203	-1.8401419	0.8143757
O	1.7848430	-2.0722414	-0.0605970
C	1.2379762	-3.3880986	0.0872880
C	-0.0046887	-3.4714933	-0.7652876
O	-0.9260930	-2.4858238	-0.2817230
C	-3.1687795	-1.7602207	-0.0102908
C	-2.2435828	-2.6260476	-0.8297801
H	-3.5232612	2.1434574	-0.5979046
H	-4.5149477	0.3224113	0.6847899
H	-2.0217728	4.0337868	-0.1986663
H	-0.1958122	3.2266868	-1.6087828
H	2.1649800	2.3209962	-1.6866578
H	4.1543208	1.7203630	-0.4114260
H	4.0805487	-0.7272829	-0.6121038
H	3.6135095	-2.6784660	0.7705347
H	1.9687739	-4.1506110	-0.2395470
H	0.2368619	-3.2889497	-1.8287793
H	-4.2044878	-1.8556933	-0.3858979
H	-2.2566563	-2.3211449	-1.8925056
H	-3.1276369	0.2635190	1.8153802
H	-3.1484434	-2.0872544	1.0461514
H	-2.5798548	-3.6769252	-0.7656585
H	-0.4390527	-4.4838463	-0.6759379
H	0.9809560	-3.5803598	1.1458240
H	2.5395070	-1.7468787	1.8587035
H	4.3611565	-0.3102806	1.1104752
H	3.3882925	2.1799670	1.1430649
H	2.6288514	3.6955190	-0.6333896
H	0.4013696	4.5307954	-0.5327316
H	-1.0678333	3.7867243	1.2978354
H	-3.5300919	2.5731204	1.1443857
Na	0.0243650	0.0527864	0.0513872

18crown-6-Cs

C	-3.3975015	1.4029628	-0.3538322
C	-2.3024907	2.2695107	-0.9522719
O	-1.3735488	2.6040116	0.0882571
C	-0.4846263	3.6858278	-0.2322404
C	0.8291392	3.2396805	-0.8518505
O	1.5636474	2.5016115	0.1348835
C	2.9426660	2.2751046	-0.1995031
C	3.1946883	0.9432344	-0.8848525
O	2.9378609	-0.1042447	0.0615256
C	3.3960915	-1.4024928	-0.3519689
C	2.3015274	-2.2711395	-0.9480778
O	1.3736354	-2.6045626	0.0937022
C	0.4843065	-3.6865047	-0.2250265

C	-0.8286105	-3.2412663	-0.8471154
O	-1.5638557	-2.5001292	0.1368185
C	-2.9425608	-2.2743779	-0.1995454
C	-3.1940625	-0.9427185	-0.8854706
O	-2.9406080	0.1049178	0.0616294
Cs	-0.0014613	0.0018185	1.5281481
H	-3.7888301	1.9005051	0.5460321
H	-2.7649118	3.1908723	-1.3546251
H	-4.2508593	-0.9105504	-1.2119371
H	-3.5003532	-2.2945552	0.7482514
H	-1.3969446	-4.1427573	-1.1461697
H	0.2703816	-4.1973359	0.7254688
H	2.7644750	-3.1928449	-1.3490844
H	3.7887302	-1.8981740	0.5483756
H	4.2523014	0.9103110	-1.2085602
H	3.4989316	2.2951736	0.7491791
H	-0.2719315	4.1992183	0.7171629
H	1.3973775	4.1406123	-1.1528085
H	-1.8004247	1.7498997	-1.7912666
H	-0.9817591	4.4049027	-0.9078357
H	0.6553482	2.6322862	-1.7611353
H	3.3222932	3.0929232	-0.8371911
H	2.5615677	0.8346417	-1.7866780
H	4.2219856	-1.3053251	-1.0779585
H	1.7984817	-1.7534003	-1.7876382
H	0.9816705	-4.4076067	-0.8983160
H	-0.6537073	-2.6364462	-1.7578988
H	-3.3208291	-3.0924201	-0.8377125
H	-2.5586579	-0.8336163	-1.7856420
H	-4.2241471	1.3054562	-1.0789591

18crown-6-NaNO3

C	-3.0982076	1.8664033	0.0123074
C	-3.3894684	0.5832951	0.7571809
O	-2.9074893	-0.5078894	-0.0306280
O	-1.6901478	1.9616908	-0.2475198
C	-1.2710819	3.3106565	-0.4482682
C	0.1502124	3.3215918	-0.9680076
O	0.9724525	2.5929288	-0.0624103
C	2.3698045	2.8208480	-0.2726904
C	3.1448374	1.8005969	0.5274276
O	2.9613719	0.5315385	-0.1052766
C	3.4615246	-0.5520847	0.6815338
C	3.1527952	-1.8422485	-0.0436963
O	1.7387675	-1.9406846	-0.2683575
C	1.3154548	-3.2920316	-0.4424090
C	-0.1175917	-3.3094189	-0.9283807
O	-0.9188826	-2.5705857	-0.0122430
C	-3.0770197	-1.7708283	0.6183295
C	-2.3206543	-2.7992717	-0.1891155
H	-3.6501406	1.9045951	-0.9455203
H	-4.4852828	0.5052002	0.9111221
H	-1.9190291	3.8186294	-1.1898315
H	0.2000532	2.8707045	-1.9786844

H	2.6208558	2.7184758	-1.3458299
H	4.2175807	2.0794976	0.5391406
H	4.5606645	-0.4729472	0.8089181
H	3.6813042	-1.8895672	-1.0142831
H	1.9457898	-3.8091544	-1.1927172
H	-0.1913372	-2.8701879	-1.9427785
H	-4.1493405	-2.0488631	0.6569530
H	-2.5955673	-2.7069725	-1.2573589
H	-2.8882417	0.5881066	1.7407647
H	-2.6784825	-1.7313057	1.6478989
H	-2.5851818	-3.8183342	0.1535603
H	-0.4508851	-4.3644826	-0.9872518
H	1.3982510	-3.8372737	0.5169403
H	3.5021701	-2.6819184	0.5860122
H	2.9835137	-0.5473518	1.6765551
H	2.7697956	1.7709607	1.5660503
H	2.6409832	3.8432627	0.0543889
H	0.4822255	4.3757805	-1.0468430
H	-1.3311997	3.8677382	0.5058970
H	-3.4318968	2.7122868	0.6421637
Na	0.0307993	0.0134886	0.5220413
N	0.0656881	0.0289097	3.3464335
O	0.0810151	0.0370993	4.5836874
O	1.1269807	0.2744753	2.6558387
O	-1.0125742	-0.2259968	2.6858452

18crown-6-CsNO3

C	-3.3925058	1.3634185	-0.2743527
C	-2.3175964	2.2483227	-0.8875738
O	-1.3877145	2.5975174	0.1382913
C	-0.4802184	3.6447664	-0.2163947
C	0.8117305	3.1595317	-0.8565407
O	1.5775828	2.4816303	0.1394007
C	2.9356100	2.2252603	-0.2308381
C	3.1501332	0.8875266	-0.9228469
O	2.9629157	-0.1486498	0.0409278
C	3.4138200	-1.4399596	-0.3778701
C	2.3339052	-2.2946184	-1.0242719
O	1.4085734	-2.6884943	-0.0105686
C	0.4971888	-3.7166414	-0.4100846
C	-0.8016976	-3.1966554	-1.0072993
O	-1.5542838	-2.5737955	0.0337138
C	-2.9192762	-2.3054717	-0.3013029
C	-3.1490312	-0.9384808	-0.9277677
O	-2.9382479	0.0532435	0.0770418
Cs	0.0274570	-0.1057441	1.8868809
H	-3.7369809	1.8325576	0.6590374
H	-2.8001343	3.1626030	-1.2883946
H	-4.1945070	-0.8935104	-1.2939689
H	-3.4810943	-2.3537558	0.6426517
H	-1.3652508	-4.0565650	-1.4226392
H	0.2587167	-4.2858344	0.5004737
H	2.8131524	-3.1902147	-1.4687171
H	3.7664574	-1.9532709	0.5288728

H	4.1866848	0.8588241	-1.3149780
H	3.5143450	2.2290131	0.7040805
H	-0.2306325	4.1636603	0.7208694
H	1.3697278	4.0416610	-1.2308970
H	-1.8201006	1.7334000	-1.7336473
H	-0.9725601	4.3683308	-0.8938612
H	0.6000818	2.5047249	-1.7253138
H	3.3160498	3.0363925	-0.8801324
H	2.4630449	0.7740224	-1.7850925
H	4.2665879	-1.3418397	-1.0754214
H	1.8321780	-1.7417657	-1.8434052
H	0.9812892	-4.4022419	-1.1314549
H	-0.5992359	-2.4954522	-1.8413218
H	-3.3089069	-3.0876908	-0.9799923
H	-2.4821064	-0.7858914	-1.7996537
H	-4.2512989	1.2991359	-0.9683255
N	0.0492944	-0.1971197	5.3578833
O	0.0564295	-0.2576879	6.6033237
O	1.1514946	-0.1659710	4.6937127
O	-1.0599065	-0.1658591	4.7059746

Calix4-biscrown6 arene-CsNO3

C	-1.1432641	-1.6006342	-6.8460768
C	-0.0895512	-0.5972569	-7.2721108
O	0.9246812	-0.4795070	-6.2837452
C	1.9438669	0.4253807	-6.6917327
C	3.1513493	0.3262720	-5.7843226
O	2.9301992	1.0062880	-4.5566767
C	4.0619877	0.9055003	-3.7056531
C	3.8162767	1.6127369	-2.3909066
O	2.8479699	0.8975031	-1.6088160
C	2.9545252	1.0856768	-0.2380370
C	3.3871281	-0.0133062	0.5346539
C	3.6147699	0.1847983	1.9024342
C	3.3946690	1.4241456	2.5022825
C	2.8678424	2.4633191	1.7374161
C	2.6126995	2.3155152	0.3664120
C	3.6403140	-1.3797637	-0.0826677
C	2.4604555	-2.0213667	-0.7980959
C	1.2457961	-2.3491632	-0.1615929
C	0.1267651	-2.7920385	-0.8921851
C	0.2723970	-3.0033933	-2.2680495
C	1.4901529	-2.7806201	-2.9027211
C	2.5615158	-2.2795278	-2.1704777
O	1.1104145	-2.2345558	1.2264428
C	1.7436847	-3.3123218	1.9429800
C	1.1103332	-3.4945704	3.3056640
O	1.3819905	-2.3637432	4.1221278
C	1.2182253	-2.5931112	5.5287712
C	-0.2259743	-2.8338818	5.9660442
O	-1.0886711	-1.7110893	5.8011521
C	-1.0216355	-0.7915598	6.9021016
C	-2.0947272	0.2614936	6.7514018
C	-1.2194766	-3.0634830	-0.2395411

C	-1.9281407	-1.8710455	0.3859230
C	-2.2111024	-0.6992376	-0.3493109
C	-2.7362965	0.4538217	0.2821151
C	-3.1324956	0.3426739	1.6226133
C	-2.9795593	-0.8481362	2.3318942
C	-2.3457397	-1.9289930	1.7211895
C	1.9588440	3.4656987	-0.3883188
C	0.6718538	3.1295875	-1.1243029
C	0.6195558	3.2071279	-2.5209027
C	-0.5439811	2.8986413	-3.2202735
C	-1.6638544	2.4544058	-2.5238682
C	-1.6587422	2.3422706	-1.1276605
C	-0.4990639	2.7478739	-0.4401208
C	-2.8837672	1.8083471	-0.4041611
O	-0.5049142	2.7879383	0.9568275
C	-1.0133281	4.0490592	1.4477642
C	-0.8679976	4.1497028	2.9470986
O	-1.7340665	3.2233300	3.5986757
C	-1.7677433	3.4686687	5.0132553
C	-2.5215948	2.3651731	5.7173657
O	-1.7474889	1.1668082	5.7062617
O	-1.8848197	-0.6923987	-1.6925575
C	-2.9890875	-0.6445664	-2.6123283
C	-3.6348395	-2.0064470	-2.8589106
O	-2.8403337	-2.8642584	-3.6819612
C	-3.2797472	-2.9835084	-5.0310854
C	-3.3129520	-1.6894450	-5.8521423
O	-2.0850626	-0.9853254	-5.9689663
H	3.5524241	1.5619549	3.5724111
H	-3.3007589	-0.9169553	3.3718977
H	-0.5969398	-3.3279298	-2.8413127
H	1.5914719	-2.9537353	-3.9746317
H	-2.5693343	2.1837822	-3.0702766
H	1.5105494	3.5172065	-3.0693056
H	-0.5677250	2.9747061	-4.3075397
H	3.5068140	-2.0602568	-2.6710726
H	-0.4488575	4.8777845	0.9833927
H	-2.0741816	4.1622660	1.1612930
H	-1.1379763	5.1871854	3.2316032
H	0.1777060	3.9798857	3.2623864
H	-2.2817084	4.4321378	5.2063092
H	-0.7386212	3.5229933	5.4124629
H	-2.6931413	2.6900472	6.7610570
H	-3.5102479	2.1964074	5.2457818
H	-0.2137574	-3.1568999	7.0261645
H	-0.6778022	-3.6518329	5.3833613
H	1.8267411	-3.4695023	5.8330090
H	1.6265651	-1.6942414	6.0115305
H	2.8224699	-3.1115425	2.0653141
H	0.0221469	-3.6581396	3.1908018
H	1.5461202	-4.4077987	3.7588897
H	1.6288394	-4.2499965	1.3722927
H	4.9461151	1.3775813	-4.1850188
H	4.3101778	-0.1573342	-3.5212090
H	3.3829661	-0.7415890	-5.6013506

H	4.0210951	0.7722883	-6.3112871
H	2.2717948	0.1774134	-7.7227348
H	1.5648890	1.4658947	-6.7022035
H	-3.7073962	-1.9504641	-6.8573951
H	-4.0192368	-0.9728171	-5.4057996
H	-4.3026672	-3.4150735	-5.0676933
H	-2.5990544	-3.7156103	-5.4899500
H	-4.6343066	-1.8557145	-3.3084387
H	-3.7872781	-2.5222477	-1.8967379
H	4.7724646	1.6692802	-1.8419978
H	3.4766629	2.6437635	-2.5921163
H	-2.1687880	-2.8454156	2.2883471
H	-3.5419215	1.2235685	2.1210755
H	2.6230292	3.4099988	2.2237010
H	3.9690963	-0.6524049	2.5074018
H	4.0191627	-2.0338677	0.7177439
H	4.4572976	-1.3043528	-0.8184897
H	-1.8609828	-3.5142282	-1.0128091
H	-1.1089678	-3.8241827	0.5493976
H	-3.7106259	1.7825949	-1.1329146
H	-3.2030556	2.5156795	0.3754976
H	1.7726212	4.2618439	0.3485946
H	2.6581674	3.8977997	-1.1215353
H	-3.7678171	0.0478292	-2.2491112
H	-2.5639699	-0.2537521	-3.5457798
N	1.5223119	1.8571207	6.0674580
O	1.4356759	2.6986668	5.1095625
O	1.8601266	0.6525904	5.7897960
O	1.2638259	2.1923107	7.2405703
H	-1.2040670	-1.3410497	7.8469230
H	-3.0759526	-0.2139594	6.5519346
H	-0.6494963	-2.4656099	-6.3675746
H	0.3601735	-0.9418415	-8.2270713
H	-2.1657580	0.8124982	7.7085669
H	-0.0317012	-0.3041857	6.9603542
H	-1.6687108	-1.9616766	-7.7528453
H	-0.5748601	0.3801660	-7.4636145
Cs	0.1879198	0.4594596	3.2423448

Calix4-biscrown6 arene-NaNO3

C	-1.1932385	-1.5761432	-6.6228537
C	-0.1388618	-0.5640505	-7.0284226
O	0.8886236	-0.4827967	-6.0499877
C	1.9126627	0.4205869	-6.4482703
C	3.1269251	0.2913916	-5.5532658
O	2.9253489	0.9597312	-4.3159928
C	4.0565624	0.8259321	-3.4687644
C	3.8198882	1.5163156	-2.1429007
O	2.8442360	0.7959845	-1.3764448
C	2.9120768	0.9724822	-0.0023319
C	3.3001918	-0.1432056	0.7695098
C	3.4519508	0.0238089	2.1507882
C	3.2087172	1.2526252	2.7635797
C	2.7392375	2.3138337	1.9921409

C	2.5586456	2.1960185	0.6077819
C	3.5825522	-1.4965580	0.1391299
C	2.4168554	-2.1407784	-0.5936970
C	1.1972148	-2.4537714	0.0360931
C	0.0833326	-2.9076509	-0.6942509
C	0.2389988	-3.1367352	-2.0663916
C	1.4627776	-2.9242860	-2.6945684
C	2.5310716	-2.4159479	-1.9616250
O	1.0594991	-2.2977406	1.4202957
C	1.5810984	-3.4098952	2.1579757
C	1.0179001	-3.4292315	3.5622207
O	1.4922436	-2.3095331	4.3173469
C	1.4999320	-2.5260747	5.7363584
C	0.1246742	-2.4603334	6.3807071
O	-0.4273885	-1.1645702	6.1585709
C	-1.5273944	-0.8772335	7.0287313
C	-1.9245532	0.5770862	6.9231942
C	-1.2702479	-3.1512276	-0.0461736
C	-1.9109686	-1.9393462	0.6084835
C	-2.2302124	-0.7779506	-0.1252737
C	-2.6782231	0.3962115	0.5230424
C	-2.9069963	0.3385347	1.9030472
C	-2.6935567	-0.8300949	2.6319816
C	-2.1819229	-1.9501935	1.9815517
C	1.9567723	3.3678582	-0.1532406
C	0.6665269	3.0630727	-0.8949787
C	0.6154679	3.1612623	-2.2902855
C	-0.5470112	2.8589210	-2.9944316
C	-1.6663551	2.4030765	-2.3038803
C	-1.6609520	2.2784065	-0.9090665
C	-0.5021413	2.6711236	-0.2133064
C	-2.8775202	1.7309841	-0.1848527
O	-0.5061747	2.6596946	1.1809741
C	-0.9508827	3.9159902	1.7287290
C	-0.9374474	3.8837223	3.2398949
O	-1.9774897	3.0373149	3.7227318
C	-2.1821138	3.1811628	5.1302183
C	-3.1636027	2.1172831	5.5942820
O	-2.6153376	0.7993313	5.6951765
O	-1.9928054	-0.7958503	-1.4900037
C	-3.1436737	-0.7425603	-2.3457907
C	-3.7331598	-2.1176450	-2.6481744
O	-2.9037774	-2.9141542	-3.4979451
C	-3.3309346	-3.0019434	-4.8524020
C	-3.3663892	-1.6882842	-5.6422041
O	-2.1403732	-0.9783051	-5.7397244
H	3.3604571	1.3654408	3.8380397
H	-2.8864622	-0.8412918	3.7051121
H	-0.6281858	-3.4622524	-2.6426587
H	1.5706860	-3.1099982	-3.7637884
H	-2.5699815	2.1315018	-2.8534024
H	1.5081596	3.4761043	-2.8337354
H	-0.5691982	2.9454463	-4.0810345
H	3.4805338	-2.2039050	-2.4579000
H	-0.2853594	4.7305227	1.3866677

H	-1.9702493	4.1447188	1.3686930
H	-1.0976272	4.9236076	3.5927518
H	0.0418986	3.5450153	3.6241184
H	-2.6124894	4.1820223	5.3454577
H	-1.2224975	3.0973046	5.6698194
H	-3.5884816	2.4195697	6.5710324
H	-3.9894503	2.0459938	4.8708956
H	0.2507541	-2.6411207	7.4660178
H	-0.5581379	-3.2414006	5.9916755
H	1.9607807	-3.5057457	5.9640191
H	2.1286194	-1.7244571	6.1476058
H	2.6845827	-3.3674588	2.2022836
H	-0.0850259	-3.4340527	3.5266723
H	1.3538001	-4.3669345	4.0438317
H	1.2978599	-4.3565043	1.6624455
H	4.9482490	1.2905933	-3.9414930
H	4.2860272	-0.2440279	-3.3009565
H	3.3426483	-0.7821664	-5.3850554
H	3.9994023	0.7303660	-6.0819251
H	2.2283989	0.1911832	-7.4875297
H	1.5441528	1.4648786	-6.4334970
H	-3.7572649	-1.9269288	-6.6548012
H	-4.0761920	-0.9851446	-5.1802270
H	-4.3502434	-3.4403286	-4.9092686
H	-2.6408394	-3.7167159	-5.3246179
H	-4.7364575	-1.9881079	-3.0971962
H	-3.8672390	-2.6745743	-1.7063637
H	4.7758580	1.5553455	-1.5917263
H	3.4901343	2.5530225	-2.3306076
H	-1.9807896	-2.8649481	2.5442833
H	-3.2155264	1.2481318	2.4194240
H	2.4939752	3.2628210	2.4737297
H	3.7778760	-0.8254782	2.7551069
H	3.9551818	-2.1573305	0.9376842
H	4.4080881	-1.4029477	-0.5844258
H	-1.9282007	-3.5594474	-0.8279339
H	-1.1855810	-3.9336999	0.7255808
H	-3.6986217	1.6706747	-0.9165835
H	-3.2148954	2.4439080	0.5823968
H	1.7910025	4.1725418	0.5796088
H	2.6750777	3.7750136	-0.8818531
H	-3.9373965	-0.1209404	-1.8966679
H	-2.7933654	-0.2686017	-3.2726587
N	1.8405578	1.6317058	6.2849854
O	0.8257702	2.0325316	5.5939988
O	2.4251564	0.5601650	5.8947468
O	2.2208796	2.2572235	7.2789587
H	-2.3891187	-1.5272070	6.7841655
H	-2.5931444	0.8111110	7.7762338
H	-0.6987150	-2.4475800	-6.1569918
H	0.2983958	-0.8792848	-7.9993213
H	-1.0257964	1.2152110	6.9982277
H	-1.2247716	-1.0816452	8.0732758
H	-1.7145769	-1.9235741	-7.5375054
H	-0.6216899	0.4210767	-7.1823183

Na 0.6903046 0.0905780 4.2815800

Calix4-biscrown6 arene

C	1.2521126	-1.5449581	2.2903128
C	2.2030945	-0.5076280	2.3060730
C	3.3746350	-0.6739996	1.5591597
C	3.5895295	-1.8207993	0.8013168
C	2.6033998	-2.8009263	0.7404818
C	1.4130254	-2.6760936	1.4647626
C	1.9695356	0.7843682	3.0725216
C	0.8601004	1.6681473	2.5232390
C	-0.2598634	1.9538470	3.3093984
C	-1.2881334	2.7662325	2.8389916
C	-1.2320524	3.2387802	1.5312771
C	-0.1549436	2.9494531	0.6805086
C	0.9340623	2.2328440	1.2311218
C	-0.2425935	3.3726168	-0.7845720
C	-0.2077355	2.2287101	-1.7949863
C	0.8530556	2.1748147	-2.7104474
C	1.0334223	1.0953430	-3.5693671
C	0.1537043	0.0188892	-3.4969821
C	-0.9460585	0.0345384	-2.6348218
C	-1.1564646	1.1799843	-1.8363988
C	-1.8928720	-1.1548919	-2.5906452
C	-1.9757046	-1.8677559	-1.2495722
C	-0.8849679	-2.5834169	-0.7198757
C	-0.9214025	-3.1179767	0.5847621
C	-2.1183093	-3.0237886	1.3035916
C	-3.2344623	-2.3898801	0.7650566
C	-3.1496326	-1.7957233	-0.4905332
O	0.2639408	-2.6970590	-1.5008006
C	0.3085029	-3.6996506	1.2626843
O	-2.3131494	1.1884997	-1.0791770
O	2.1073876	2.0077968	0.5345801
O	0.1066550	-1.3958889	3.0703137
H	-2.1551821	-3.4177879	2.3204676
H	-4.1513849	-2.3115268	1.3503343
H	-0.3105720	1.5376747	4.3171523
H	-2.0560035	3.8436866	1.1465802
H	-2.1471149	2.9942871	3.4703356
H	4.1069809	0.1339298	1.5426491
H	2.7348473	-3.6618304	0.0829970
H	-1.5744430	-1.8564450	-3.3764254
H	-2.9111324	-0.8280843	-2.8530634
H	0.5774594	4.0566400	-1.0490374
H	1.7257004	0.5670011	4.1240851
H	2.9196105	1.3401017	3.0765760
H	-0.0159210	-4.1334301	2.2211398
H	0.7304840	-4.5325584	0.6796556
H	-3.9941981	-1.2273421	-0.8817975
H	4.4995320	-1.9269622	0.2097434
H	0.3070049	-0.8549616	-4.1329508
H	1.8770580	1.0763680	-4.2597414
H	1.5641853	3.0033277	-2.7363945

H	-1.1620307	3.9678630	-0.8912325
C	2.8185594	3.1582344	0.0578114
C	0.3900568	-3.9617642	-2.1616836
H	2.6697888	3.2581340	-1.0287775
C	4.3056046	3.0253435	0.3236155
H	2.4484403	4.0698028	0.5569940
H	0.6652643	-4.7576137	-1.4454766
C	1.4295789	-3.8873135	-3.2594177
H	-0.5757647	-4.2442162	-2.6205931
H	4.5035148	2.8987406	1.4075283
H	4.7869023	3.9733063	0.0024468
H	1.2110994	-3.0338934	-3.9295635
H	1.3488675	-4.8184307	-3.8592851
O	4.8253186	1.9279490	-0.4092566
C	6.2439508	1.8963801	-0.4211347
O	2.7404157	-3.7643256	-2.7239482
C	3.7275555	-3.8882359	-3.7416241
H	6.6475899	1.9802561	0.6097390
H	6.6438415	2.7448600	-1.0122123
C	6.7238697	0.5848077	-1.0077707
C	5.1103235	-3.6141867	-3.1839474
H	3.5304488	-3.1796270	-4.5692624
H	3.6997743	-4.9147042	-4.1622738
H	6.2645204	-0.2499776	-0.4472219
H	7.8241032	0.5249130	-0.8716088
H	5.8588482	-4.1724957	-3.7833520
H	5.1683730	-3.9885370	-2.1430552
O	6.3948922	0.5213381	-2.3886839
C	7.0895518	-0.4911940	-3.1026219
O	5.3993204	-2.2214106	-3.2444735
C	6.7125585	-1.9346381	-2.7885084
H	8.1832908	-0.3898111	-2.9363556
H	7.4481803	-2.5858687	-3.3078338
H	6.8824262	-0.2956971	-4.1647386
H	6.8062216	-2.1491635	-1.7047701
C	-3.2004795	2.3019974	-1.2474735
C	0.1535058	-2.1155853	4.3084169
H	-2.9643182	2.8401392	-2.1812165
H	-3.0917289	2.9938761	-0.3977937
C	-4.6428770	1.8384488	-1.3015843
H	0.0101477	-3.1991216	4.1415108
C	-0.9054762	-1.6057398	5.2617380
H	1.1413266	-1.9778288	4.7861703
H	-4.7936921	1.1142311	-2.1281152
H	-5.2717695	2.7283192	-1.5165025
H	-0.8233138	-0.5064670	5.3652264
H	-0.7028271	-2.0551215	6.2572943
O	-5.0055635	1.2596017	-0.0587952
C	-6.4023061	1.0375171	0.0557693
O	-2.2107950	-1.9578332	4.8241145
C	-3.1858440	-1.6434420	5.8120400
H	-6.7843456	0.4806678	-0.8252856
H	-6.9435822	2.0033827	0.1074381
C	-6.6929715	0.2144185	1.2938275
C	-4.5851353	-1.8808346	5.2806496

H	-3.0993295	-0.5855097	6.1269064
H	-3.0235636	-2.2768945	6.7087178
H	-6.0972890	-0.7157521	1.2564217
H	-7.7674563	-0.0647034	1.2804056
H	-5.2595071	-2.1114549	6.1311592
H	-4.5801237	-2.7616566	4.6091751
O	-6.3952202	0.9692066	2.4602496
C	-6.9599647	0.4394365	3.6510900
O	-5.0580303	-0.7221679	4.6021468
C	-6.3934025	-0.8846327	4.1506353
H	-8.0549012	0.3037032	3.5234536
H	-7.0421804	-1.2233105	4.9873219
H	-6.7940970	1.2073645	4.4205528
H	-6.4489647	-1.6681169	3.3677262

Calix4-biscrown6 arene-Na

C	1.2115575	-1.3928297	2.9775755
C	2.1954454	-0.4209272	3.2483473
C	3.5361999	-0.7533008	3.0099587
C	3.8924355	-1.9841892	2.4610838
C	2.8916424	-2.8878764	2.1028161
C	1.5388334	-2.6084109	2.3408573
C	1.8410381	0.9398226	3.8183684
C	0.8271656	1.7854970	3.0613980
C	-0.2620978	2.3257159	3.7573625
C	-1.1800093	3.1617740	3.1300008
C	-1.0303455	3.4520260	1.7766322
C	0.0329369	2.9315245	1.0260613
C	0.9667936	2.1184237	1.7014151
C	0.1490794	3.3253237	-0.4429292
C	0.3610927	2.1982832	-1.4394260
C	1.5155372	2.2093281	-2.2380378
C	1.8531144	1.1370895	-3.0632549
C	1.0331863	0.0065382	-3.0694793
C	-0.1570564	-0.0379292	-2.3296740
C	-0.5253456	1.0995001	-1.5719738
C	-1.0458708	-1.2656057	-2.3881668
C	-1.3292901	-1.9585715	-1.0656640
C	-0.3197323	-2.5129785	-0.2582456
C	-0.6026894	-3.0921693	0.9958963
C	-1.9436598	-3.1765248	1.3879640
C	-2.9661949	-2.6865999	0.5820015
C	-2.6529904	-2.0662013	-0.6222050
O	1.0146623	-2.4474392	-0.7118742
C	0.4681532	-3.6072389	1.9461523
O	-1.7450337	1.0428839	-0.9505697
O	2.0924416	1.6111844	1.0235331
O	-0.0990220	-1.1406836	3.3482859
H	-2.1810027	-3.6023165	2.3638283
H	-4.0016754	-2.7544862	0.9147941
H	-0.3742705	2.0938287	4.8182977
H	-1.7487408	4.1111894	1.2853573
H	-2.0144321	3.5837787	3.6908546
H	4.3120286	-0.0377315	3.2908185

H	3.1615674	-3.8491766	1.6601281
H	-0.5866839	-1.9709181	-3.0974297
H	-2.0181933	-0.9846436	-2.8208550
H	0.9852129	4.0320225	-0.5689974
H	1.4572378	0.8251609	4.8442702
H	2.7812269	1.5056835	3.9220829
H	-0.0525630	-3.9690314	2.8455630
H	0.9754338	-4.4917088	1.5298465
H	-3.4449860	-1.6353033	-1.2353885
H	4.9427475	-2.2409190	2.3158875
H	1.3170121	-0.8611151	-3.6666486
H	2.7681271	1.1570418	-3.6529650
H	2.1764291	3.0774010	-2.1915636
H	-0.7503823	3.9076648	-0.6900758
C	3.1547079	2.5777604	0.8532953
C	1.5757081	-3.7338520	-1.0848756
H	2.9513034	3.2016733	-0.0315673
C	4.4834424	1.8772537	0.6939680
H	3.2030441	3.2310824	1.7395065
H	2.5895309	-3.7814936	-0.6596103
C	1.6497222	-3.9525514	-2.5811018
H	0.9660632	-4.5341890	-0.6425415
H	4.7375177	1.2999899	1.6004216
H	5.2540084	2.6581002	0.5580595
H	0.6800218	-3.7087419	-3.0556221
H	1.8453895	-5.0290833	-2.7633332
O	4.4664236	1.0107129	-0.4459809
C	5.8068205	0.6790864	-0.8495785
O	2.7050968	-3.1674014	-3.1211728
C	2.8270884	-3.3160058	-4.5377262
H	6.2919273	0.0581194	-0.0720666
H	6.3839032	1.6145508	-0.9570786
C	5.8283591	-0.0699403	-2.1625950
C	4.1925968	-2.8465209	-4.9828258
H	2.0319574	-2.7461373	-5.0556757
H	2.7190222	-4.3803254	-4.8213144
H	5.2385540	-1.0049568	-2.1018027
H	6.8836050	-0.3539919	-2.3439577
H	4.3187435	-3.0793383	-6.0587426
H	4.9699067	-3.4025345	-4.4233423
O	5.3337826	0.7666848	-3.1983148
C	5.8018666	0.4460418	-4.5114216
O	4.3282288	-1.4488211	-4.7501836
C	5.6701080	-1.0134584	-4.9162657
H	6.8680340	0.7286619	-4.6194550
H	5.9970935	-1.1053107	-5.9719350
H	5.2103924	1.0819990	-5.1841122
H	6.3472629	-1.6527028	-4.3158414
C	-2.6543711	2.1503887	-1.1502798
C	-0.3840528	-1.6276644	4.6806676
H	-2.3024267	2.7754412	-1.9860369
H	-2.6935104	2.7491596	-0.2280204
C	-4.0443030	1.6422897	-1.4676616
H	-0.3933341	-2.7316703	4.6871764
C	-1.7050011	-1.1016590	5.1941891

H	0.4139259	-1.2933959	5.3670563
H	-4.0124020	0.9508996	-2.3353248
H	-4.6651139	2.5144180	-1.7642285
H	-1.7707198	-0.0097190	5.0233347
H	-1.7106249	-1.2730331	6.2903752
O	-4.5819358	1.0055056	-0.3275133
C	-5.9042964	0.5203872	-0.5487380
O	-2.8077425	-1.7662011	4.5944367
C	-4.0010743	-1.5504333	5.3484979
H	-5.9095014	-0.2015056	-1.3912894
H	-6.5826255	1.3548409	-0.8129901
C	-6.4051700	-0.1739999	0.6958906
C	-5.2087113	-2.1486975	4.6419017
H	-4.1559211	-0.4685580	5.5247865
H	-3.9013336	-2.0319715	6.3431047
H	-5.6360087	-0.8676533	1.0760897
H	-7.3049071	-0.7660014	0.4339628
H	-6.0080022	-2.2869447	5.3968478
H	-4.9423820	-3.1384798	4.2437315
O	-6.7388522	0.8065556	1.6762610
C	-7.3451622	0.2684804	2.8462401
O	-5.7171472	-1.4026215	3.5395242
C	-6.3698401	-0.1886414	3.9212867
H	-8.0263013	-0.5633713	2.5850744
H	-5.6336148	0.6147880	4.1060426
H	-7.9500040	1.0844032	3.2733280
H	-6.9445342	-0.3498850	4.8563289
Na	2.2437940	-0.2613526	-0.5334074

Calix4-biscrown6 arene-Cs

C	1.2647327	-1.5196318	2.3969792
C	2.2644054	-0.5352729	2.5402595
C	3.5605376	-0.8416391	2.1036326
C	3.8490141	-2.0694327	1.5062926
C	2.8123580	-2.9688872	1.2499231
C	1.4993206	-2.7040686	1.6633611
C	1.9799045	0.8018398	3.2034808
C	0.8649692	1.6497289	2.6093059
C	-0.2278170	2.0028194	3.4099722
C	-1.2441225	2.8220995	2.9301927
C	-1.2038889	3.2558754	1.6081936
C	-0.1538546	2.9061988	0.7484182
C	0.9094563	2.1539522	1.2951082
C	-0.2076804	3.3636462	-0.7068516
C	-0.1672519	2.2665168	-1.7638735
C	0.8242464	2.3118871	-2.7559502
C	0.9613923	1.2974727	-3.7028514
C	0.1438153	0.1688579	-3.6125189
C	-0.8744216	0.0793462	-2.6556364
C	-1.0862149	1.1889514	-1.8031988
C	-1.7646585	-1.1530123	-2.5939752
C	-1.8485106	-1.8380972	-1.2374932
C	-0.7619375	-2.5289911	-0.6709261
C	-0.8174465	-3.0669048	0.6292286

C	-2.0312226	-2.9806790	1.3199757
C	-3.1405288	-2.3581183	0.7572710
C	-3.0372983	-1.7746684	-0.5011520
O	0.4065855	-2.6701840	-1.4427742
C	0.3859859	-3.6837847	1.3250526
O	-2.2067543	1.1515302	-1.0136425
O	2.0562057	1.8847536	0.5424060
O	0.0381391	-1.2978853	2.9983273
H	-2.0960410	-3.3793860	2.3328905
H	-4.0687370	-2.2877135	1.3240963
H	-0.2583906	1.6439260	4.4402098
H	-2.0078940	3.8890452	1.2284831
H	-2.0737422	3.1100835	3.5760337
H	4.3534500	-0.1062908	2.2526593
H	3.0192761	-3.9051521	0.7267205
H	-1.4070627	-1.8561753	-3.3613480
H	-2.7897168	-0.8742224	-2.8833453
H	0.6224154	4.0519668	-0.9267037
H	1.7291188	0.6379207	4.2635279
H	2.9207093	1.3734511	3.2020078
H	0.0195930	-4.1743274	2.2405158
H	0.8303637	-4.4870112	0.7177505
H	-3.8844612	-1.2278213	-0.9152340
H	4.8742491	-2.3186876	1.2256179
H	0.2647858	-0.6509442	-4.3249787
H	1.7064410	1.3817648	-4.4961435
H	1.4914597	3.1766198	-2.7907740
H	-1.1180448	3.9714142	-0.8176414
C	2.8495041	3.0424935	0.2066468
C	0.4660349	-3.9529619	-2.0992714
H	2.7453616	3.2502876	-0.8712679
C	4.3131442	2.8214049	0.5225229
H	2.4926490	3.9185990	0.7708422
H	0.7950126	-4.7302948	-1.3880609
C	1.4052432	-3.9125480	-3.2802916
H	-0.5384405	-4.2286750	-2.4630022
H	4.4662542	2.6211965	1.5994942
H	4.8513186	3.7550865	0.2702000
H	1.0908309	-3.1360736	-4.0039083
H	1.3422428	-4.8931456	-3.7901094
O	4.8167064	1.7366831	-0.2574505
C	6.2329859	1.7948784	-0.4270883
O	2.7460103	-3.6686901	-2.8516436
C	3.6829666	-3.9445109	-3.8943820
H	6.7452717	1.8503236	0.5527536
H	6.5021933	2.6955567	-1.0101901
C	6.7022586	0.5509101	-1.1483032
C	5.0842581	-3.6228397	-3.4339642
H	3.4450676	-3.3497103	-4.7973910
H	3.6338128	-5.0154901	-4.1697079
H	6.4812006	-0.3454148	-0.5384127
H	7.8000300	0.6122826	-1.2711038
H	5.7964430	-4.0312078	-4.1761095
H	5.2903895	-4.1100439	-2.4617823
O	6.0597861	0.4781368	-2.4204700

C	6.7452455	-0.3264539	-3.3811279
O	5.2449555	-2.2056644	-3.3353238
C	6.6108240	-1.8252829	-3.1722010
H	7.8206555	-0.0666452	-3.3976170
H	7.2402804	-2.3336939	-3.9284354
H	6.3107743	-0.0563455	-4.3540243
H	6.9849926	-2.1325217	-2.1760154
C	-3.1359718	2.2520264	-1.1461706
C	-0.0673985	-1.9650599	4.2764462
H	-2.8871808	2.8462389	-2.0396718
H	-3.0658096	2.8870992	-0.2513962
C	-4.5574442	1.7440916	-1.2686139
H	-0.1504594	-3.0564958	4.1351191
C	-1.2537692	-1.4624938	5.0683573
H	0.8472580	-1.7683605	4.8635920
H	-4.6471125	1.0357283	-2.1184723
H	-5.2068965	2.6156673	-1.4964397
H	-1.2571191	-0.3559908	5.0883721
H	-1.1149631	-1.8160560	6.1109654
O	-4.9416643	1.1338246	-0.0531143
C	-6.3115302	0.7375239	-0.0442861
O	-2.4810117	-1.9528000	4.5487098
C	-3.5497561	-1.7335264	5.4684271
H	-6.5156565	0.0413836	-0.8829059
H	-6.9671114	1.6213156	-0.1668509
C	-6.6268252	0.0367027	1.2570295
C	-4.8777968	-2.1903729	4.8809964
H	-3.5992102	-0.6650368	5.7547087
H	-3.3642577	-2.3109705	6.3978225
H	-5.8727209	-0.7425004	1.4578915
H	-7.6143435	-0.4574548	1.1610323
H	-5.5875764	-2.3246968	5.7216703
H	-4.7417535	-3.1663116	4.3927547
O	-6.6631214	0.9959777	2.3105981
C	-7.0673094	0.4620320	3.5659689
O	-5.4574326	-1.3367578	3.8989354
C	-5.9381125	-0.0955472	4.4224774
H	-7.8442937	-0.3135423	3.4278065
H	-5.1224670	0.6484606	4.4793160
H	-7.5173966	1.3014343	4.1199900
H	-6.3359411	-0.2478303	5.4463950
Cs	2.8867560	-0.5796876	-1.4742764

Cs-6H2O-A

O	-2.9021681	0.0041682	-1.4315927
Cs	-0.0015368	-0.0028730	-0.0001172
O	-2.8564576	-1.3303974	0.8244168
O	2.8513702	1.3282506	-0.8264516
O	-2.8785055	1.2921510	0.8527618
O	2.8766619	-1.2944862	-0.8540122
O	2.8997012	-0.0057612	1.4298657
H	-3.5009046	-0.0696410	-2.2049273

H	-3.0928936	-0.7676927	-0.8066757
H	3.4927058	-1.9732489	-1.2032558
H	3.0911299	-1.1441920	0.1222690
H	3.4988769	0.0692848	2.2027346
H	3.0886558	0.7663197	0.8046908
H	3.0461571	0.4001285	-1.1798106
H	3.4486451	1.9584207	-1.2830609
H	-3.4546115	-1.9599957	1.2806479
H	-3.0499740	-0.4020968	1.1780486
H	-3.0926738	1.1424024	-0.1236529
H	-3.4941856	1.9712980	1.2019028

Cs-6H2O-B

O	1.3862280	0.5175709	1.5186260
Cs	-1.0041385	0.8949078	-0.3405464
O	1.0778415	-0.8485270	-1.7501790
O	-3.3501974	-1.1713183	-0.1672950
O	-2.5422957	3.6251849	0.0939287
O	3.0489624	-1.3416448	0.2011754
O	5.6737482	-0.8679154	-0.3110052
H	2.0630478	-0.1132044	1.1731347
H	1.7156654	0.8030469	2.3854024
H	3.0571233	-2.2407042	0.5718620
H	4.0027635	-1.1302449	0.0028506
H	6.1257828	-0.9913584	-1.1617721
H	6.2936332	-0.3820226	0.2573796
H	-2.9687195	3.9063218	0.9211584
H	-2.6802980	4.3756331	-0.5087468
H	-3.2824640	-2.1039974	-0.4332230
H	-4.2585580	-1.0851276	0.1682631
H	1.8326381	-1.0846386	-1.1576958
H	1.3043650	-1.2228448	-2.6162834

Na-6H2O-A

O	-1.9532526	-0.0502835	-1.5329796
Na	-0.0015478	-0.0016730	-0.0007095
O	-1.8932790	-1.3612373	0.8640649
O	1.8892652	1.3595078	-0.8653738
O	-1.9267116	1.3641158	0.8074986
O	1.9242178	-1.3659557	-0.8095117
O	1.9502482	0.0479120	1.5312931
H	-2.2196725	-0.0876092	-2.4663814
H	-2.3307697	-0.8405995	-1.0915768
H	2.1755188	-2.1906920	-1.2572143
H	2.3334962	-1.3819658	0.0814369
H	2.2167936	0.0852389	2.4646577
H	2.3271600	0.8385664	1.0899712
H	2.2712329	0.5783213	-1.3200939
H	2.1237491	2.1424134	-1.3903589
H	-2.1283511	-2.1437470	1.3893779
H	-2.2748161	-0.5795834	1.3183644
H	-2.3357088	1.3801604	-0.0835792
H	-2.1775795	2.1891495	1.2548953

Na-6H₂O-B

O	0.7621025	-0.2966445	1.5289778
Na	-0.8221551	0.3257225	-0.0296737
O	0.7123554	-0.3049917	-1.6363612
O	-2.8323448	-0.8176105	0.3556955
O	-1.5757823	2.5252376	-0.3776402
O	2.8322423	-1.2086265	-0.0809191
O	5.2752250	-0.0579232	-0.1437848
H	1.6036255	-0.6372924	1.1350677
H	0.9163588	-0.2059168	2.4817327
H	3.0131821	-2.1641893	-0.0668986
H	3.7274967	-0.7660400	-0.1040239
H	5.7916850	0.1629936	-0.9361717
H	5.8319212	0.1714722	0.6183581
H	-2.1490264	3.0718897	0.1851313
H	-1.2556746	3.1273758	-1.0701877
H	-2.9150622	-1.6750798	0.8055284
H	-3.7283243	-0.6086783	0.0430431
H	1.5607683	-0.6549246	-1.2662879
H	0.7465349	-0.4476564	-2.5945518

H2O

O	0.6353512	-0.0000013	2.3616352
H	-0.1507809	0.0000005	2.9486416
H	1.3903390	0.0000005	2.9881591

 $(\text{H}_2\text{O})_6$

O	0.2959618	-0.1746630	1.6709614
H	0.6632299	0.6170242	2.1413354
H	1.0344181	-0.4287815	1.0587099
O	2.3563720	-0.3303499	-0.2257966
H	2.0475183	-0.6992417	-1.0695751
H	2.3368001	0.6533798	-0.3483841
O	-0.4036046	2.9841285	-0.7785994
H	-0.8997289	2.1303509	-0.5362191
H	-0.7673578	3.6668247	-0.1913001
O	-1.4637665	0.6818094	-0.0829549
H	-2.3711923	0.5636070	0.2378416
H	-0.8463788	0.3190018	0.6436180
O	2.0830851	2.4479863	-0.1779930
H	1.1311162	2.7013881	-0.4581197
H	2.6807624	3.0590023	-0.6382638
O	1.5744406	2.1746739	2.5487170
H	2.3694693	1.9976396	3.0773797
H	1.9034605	2.3842476	1.6375083

11 11555 1000 1155 12 170 11557 5000

Optimized Structures of different complexes at BP/TZVP level of theory

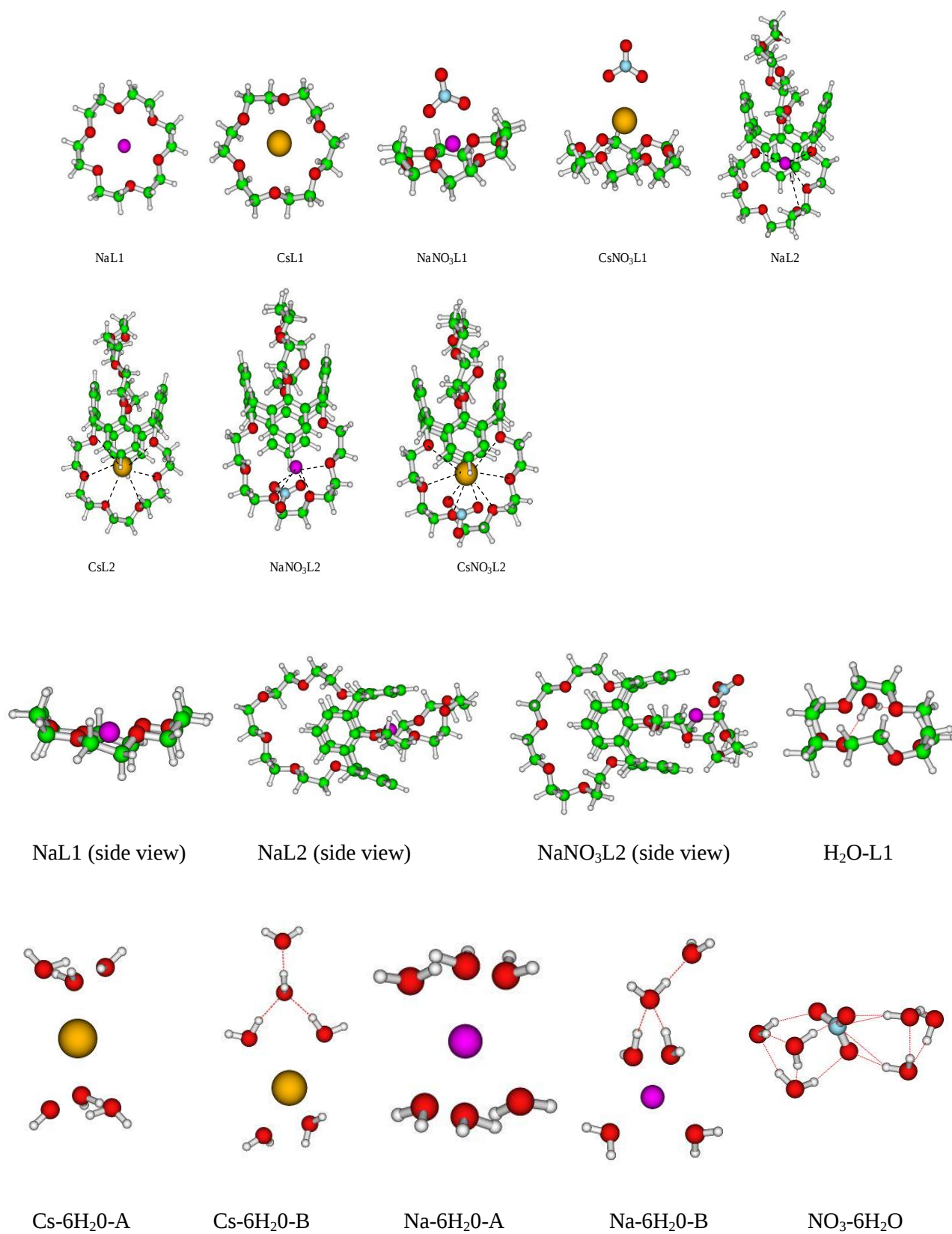


Fig.S1