

Electronic Supplementary Information

Intra-Host π - π Interactions in Crown Ether Complexes Revealed by Cryogenic Ion Mobility-Mass Spectrometry

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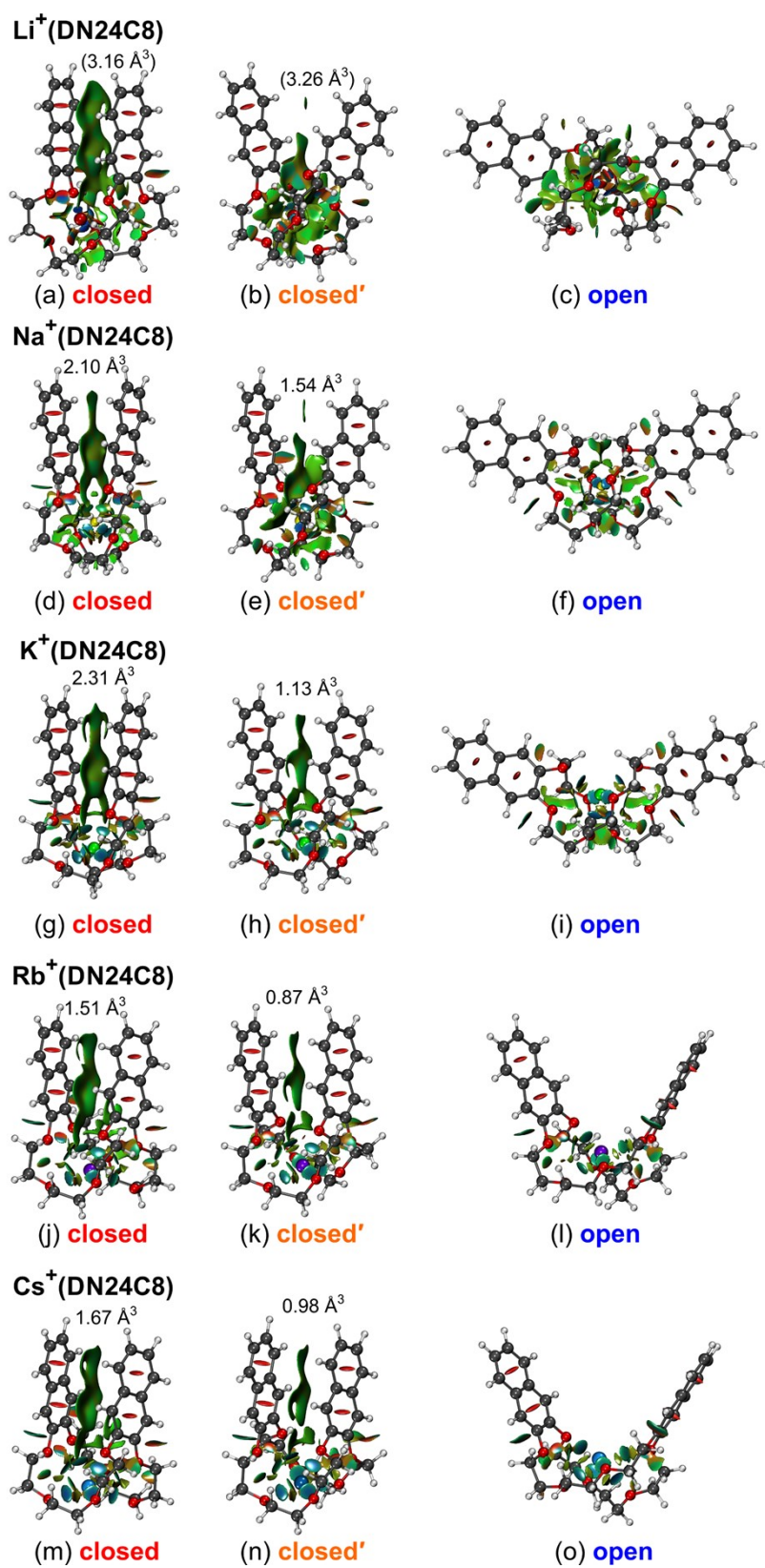


Fig. S1 Reduced density gradient (RDG) isosurfaces and the volume of the π - π interaction region between the two aromatic rings of the most stable **closed**, **closed'**, and

open conformers of $M^+(\text{DN24C8})$ ($M = \text{Li, Na, K, Rb, and Cs}$). The volume of the π - π interaction region between the two aromatic rings determined by the domain analysis is shown near the interaction region. For $\text{Li}^+(\text{DN24C8})$, the π - π interaction region between the two naphthalene rings overlapped with the host-guest interaction region. Therefore, the volumes of the π - π interaction region for the **closed** and **closed'** conformers were overestimated and were larger than that for the parallel-displaced naphthalene dimer (2.59 \AA^3).

Geometrical coordinates of conformers in Table 1.

(a) $\text{Li}^+(\text{DN24C8})$ (closed)

Li	2.015849	-0.946600	0.048504
O	3.252095	3.125326	-1.397184
O	3.143842	-2.700513	-0.297628
O	3.327428	-0.859922	1.658422
O	1.069542	2.729918	0.289136
O	0.966100	0.277655	1.420295
O	2.984919	0.301242	-1.230181
O	0.649406	-0.812573	-1.484725
O	0.470455	-2.734426	0.233087
C	4.045035	2.345506	-0.517620
C	4.362332	-2.584306	0.430023
C	4.079461	-2.058344	1.821731
C	-0.173141	2.254459	0.582714
C	-0.209545	0.989295	1.236848
C	1.058686	-3.752334	-0.594423
C	2.465750	-3.939619	-0.100961
C	2.693802	-0.422617	2.858452
C	1.796452	0.733566	2.499233
C	1.141318	3.898694	-0.523116
C	2.599730	4.212372	-0.764270
C	2.366828	0.401063	-2.514528
C	0.874532	0.330147	-2.312188
C	-0.639072	-1.174775	-1.194962
C	-0.723244	-2.251944	-0.271584
C	4.236567	0.978222	-1.120983
C	-1.389402	0.438612	1.631731
C	-1.350784	2.892844	0.294651
C	-2.619465	1.086886	1.361811
C	-1.928908	-2.738992	0.123211
C	-3.127154	-2.163544	-0.376734
C	-1.768144	-0.589019	-1.684949
C	-2.596066	2.320892	0.668234
C	-3.823337	2.962944	0.374273
C	-5.010956	2.398911	0.756594
C	-5.031139	1.168305	1.449109
C	-3.860210	0.525801	1.745215
C	-3.042236	-1.074665	-1.281318
C	-4.236821	-0.488458	-1.760787
C	-5.455876	-0.970463	-1.365729
C	-5.540057	-2.058681	-0.471219
C	-4.399986	-2.641022	0.014677

H	3.537342	2.232700	0.440359
H	5.018921	2.821309	-0.360621
H	4.983005	-1.881418	-0.120790
H	4.879776	-3.544799	0.476991
H	3.490768	-2.776096	2.400175
H	5.011231	-1.857154	2.356240
H	0.486533	-4.676547	-0.504793
H	1.061103	-3.417786	-1.632961
H	2.967300	-4.730518	-0.662843
H	2.450472	-4.202297	0.959531
H	3.439882	-0.113384	3.594385
H	2.098366	-1.244108	3.265912
H	1.172451	1.001077	3.352881
H	2.363627	1.603950	2.174516
H	0.635004	3.708584	-1.473271
H	0.661244	4.742518	-0.021104
H	3.094676	4.458911	0.177915
H	2.666043	5.079224	-1.421758
H	2.708932	-0.428679	-3.137433
H	2.619697	1.351602	-2.981020
H	0.503354	1.216868	-1.797386
H	0.368158	0.206453	-3.270720
H	4.707638	1.043992	-2.103280
H	4.872971	0.389122	-0.462926
H	-1.377695	-0.525695	2.122386
H	-1.359079	3.848982	-0.207715
H	-1.967984	-3.555815	0.832671
H	-1.721930	0.253229	-2.360382
H	-3.808974	3.909405	-0.150766
H	-5.942681	2.898674	0.530108
H	-5.976897	0.732834	1.739566
H	-3.868004	-0.422924	2.265544
H	-4.172794	0.349782	-2.442220
H	-6.362752	-0.515385	-1.739163
H	-6.509618	-2.432144	-0.172425
H	-4.457650	-3.476741	0.700297

(b) Li⁺(DN24C8) (closed')

Li	1.986626	-0.191451	0.003264
O	3.712715	1.409094	-0.236102
O	3.592520	-1.585680	-0.278980
O	2.538191	-0.603935	2.050652
O	1.260280	1.969848	0.642375
O	-0.162047	0.034599	1.634295
O	2.379560	0.182855	-2.260481
O	0.124238	-0.291761	-1.153119
O	1.033950	-2.443260	0.086924
C	4.033197	1.815878	-1.561882
C	4.410942	-1.469721	0.883677
C	3.559816	-1.593067	2.125824
C	-0.088221	2.209754	0.650014
C	-0.850008	1.136666	1.190335
C	1.785276	-2.932368	-1.037463
C	3.231588	-2.924989	-0.620209
C	1.524978	-0.847973	3.025395
C	0.467908	0.211796	2.908477
C	2.145319	3.075707	0.511936
C	3.531921	2.487968	0.672325
C	1.339234	1.077778	-2.618740

C	0.045654	0.317871	-2.443952
C	-0.815110	-1.252696	-0.864894
C	-0.321915	-2.385779	-0.168501
C	3.698370	0.660317	-2.482158
C	-2.208092	1.186858	1.196271
C	-0.702458	3.329327	0.168976
C	-2.884271	2.322512	0.676201
C	-1.168532	-3.367624	0.244306
C	-2.558289	-3.274145	-0.028502
C	-2.140854	-1.140760	-1.160963
C	-2.123935	3.408411	0.172611
C	-2.801581	4.543715	-0.330440
C	-4.170642	4.591302	-0.338831
C	-4.926736	3.507672	0.156415
C	-4.296775	2.397795	0.653752
C	-3.045836	-2.154213	-0.749723
C	-4.432288	-2.060219	-1.020164
C	-5.291192	-3.038433	-0.596056
C	-4.804971	-4.155935	0.117147
C	-3.469339	-4.271333	0.394100
H	5.097381	2.054328	-1.637030
H	3.466855	2.709537	-1.834159
H	4.860515	-0.481563	0.830732
H	5.198046	-2.226833	0.879983
H	3.093524	-2.580633	2.182731
H	4.168313	-1.440700	3.021930
H	1.461313	-3.944222	-1.286853
H	1.630625	-2.270685	-1.891426
H	3.862925	-3.275569	-1.438817
H	3.367610	-3.584181	0.238395
H	1.963889	-0.825216	4.026753
H	1.084058	-1.831391	2.842083
H	-0.273449	0.094232	3.700853
H	0.913392	1.204977	2.970131
H	2.016413	3.550675	-0.463227
H	1.941463	3.815572	1.289190
H	3.630073	2.061099	1.668339
H	4.297172	3.254335	0.528038
H	1.444884	1.407767	-3.656051
H	1.340096	1.949819	-1.961121
H	-0.801415	1.002898	-2.498409
H	-0.059312	-0.465966	-3.195798
H	3.828569	0.962559	-3.525155
H	4.345836	-0.184172	-2.263862
H	-2.766154	0.344952	1.585479
H	-0.136042	4.160918	-0.226986
H	-0.773996	-4.219862	0.782473
H	-2.523479	-0.267396	-1.672040
H	-2.222425	5.376337	-0.708500
H	-4.678269	5.464375	-0.724496
H	-6.006329	3.560118	0.145959
H	-4.869704	1.565518	1.042032
H	-4.801334	-1.204138	-1.570375
H	-6.348129	-2.960370	-0.809231
H	-5.494058	-4.922476	0.442731
H	-3.092927	-5.126802	0.939682

(c) Li⁺(DN24C8) (open)

Li	-0.011061	0.496150	0.014043
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O	1.590999	3.363600	0.104973
O	-0.992885	1.790530	-1.245389
O	-0.663226	-0.787641	-1.517424
O	1.889733	0.756086	-1.048783
O	1.180564	-1.299544	0.417621
O	0.566094	1.381147	1.840207
O	-1.482719	-0.265836	1.299752
O	-2.890321	2.000929	0.810195
C	1.860369	3.354150	1.495978
C	-1.700079	1.150754	-2.305913
C	-0.875983	-0.047152	-2.708508
C	2.924735	-0.050970	-0.650621
C	2.525700	-1.172749	0.127964
C	-2.912734	2.943911	-0.262309
C	-1.517365	3.055201	-0.843720
C	0.164214	-1.929625	-1.671313
C	0.510746	-2.373759	-0.271418
C	2.213534	1.983437	-1.717134
C	2.685984	3.027730	-0.730866
C	0.158905	0.452614	2.844791
C	-1.313131	0.209959	2.648892
C	-2.807057	-0.372190	0.916583
C	-3.540526	0.811077	0.625452
C	1.853460	1.953904	2.069588
C	3.445111	-2.059137	0.601669
C	4.249742	0.139230	-0.934549
C	4.822803	-1.891738	0.316577
C	-4.841581	0.719045	0.214368
C	-5.461554	-0.544926	0.048124
C	-3.387035	-1.598305	0.785131
C	5.225263	-0.778693	-0.461919
C	6.600712	-0.603251	-0.746741
C	7.526572	-1.494442	-0.275395
C	7.124161	-2.601624	0.503400
C	5.801149	-2.796053	0.793791
C	-4.725717	-1.721987	0.338277
C	-5.348851	-2.983745	0.181614
C	-6.646575	-3.068853	-0.243179
C	-7.381423	-1.896407	-0.529154
C	-6.804438	-0.663983	-0.386428
H	1.064696	3.933335	1.961353
H	2.817030	3.838902	1.711549
H	-1.819637	1.837193	-3.148765
H	-2.681237	0.818667	-1.960599
H	-1.412157	-0.646985	-3.448029
H	0.088920	0.262387	-3.120778
H	-3.642239	2.638743	-1.011778
H	-3.213279	3.912135	0.136388
H	-0.819232	3.427032	-0.100103
H	-1.527187	3.739692	-1.698219
H	1.069535	-1.664081	-2.226916
H	-0.367232	-2.721075	-2.206408
H	-0.395585	-2.558304	0.298094
H	1.141115	-3.261872	-0.280018
H	2.940218	1.799939	-2.508407
H	1.275630	2.311813	-2.155296
H	3.016538	3.916682	-1.273776
H	3.523666	2.651669	-0.139960
H	0.320712	0.878882	3.837534

H	0.727909	-0.473697	2.744367
H	-1.677120	-0.546716	3.345480
H	-1.870515	1.137098	2.770871
H	2.625450	1.323198	1.620012
H	2.043792	2.016297	3.144000
H	3.115724	-2.893388	1.208517
H	4.589822	0.981492	-1.518536
H	-5.413982	1.618457	0.026555
H	-2.810538	-2.483888	1.018884
H	6.910226	0.244676	-1.343829
H	8.574659	-1.353310	-0.499216
H	7.867566	-3.296015	0.868507
H	5.486569	-3.642988	1.389426
H	-4.784288	-3.878912	0.408200
H	-7.117636	-4.034917	-0.358156
H	-8.407370	-1.978039	-0.859840
H	-7.367948	0.234750	-0.600637

(d) Na⁺(DN24C8) (closed)

Na	-2.112291	0.000030	-0.000055
O	-3.529015	-1.965505	-0.427422
O	-3.528973	1.965560	0.427408
O	-2.989502	-0.024699	2.282236
O	-0.953076	-2.044992	0.521890
O	-0.233986	0.042032	1.900962
O	-2.989502	0.024708	-2.282302
O	-0.233990	-0.042020	-1.900900
O	-0.953030	2.045034	-0.521859
C	-4.008709	-2.109554	-1.758142
C	-4.008697	2.109573	1.758121
C	-4.202797	0.715548	2.314060
C	0.400582	-1.900138	0.648162
C	0.779519	-0.766386	1.423244
C	-1.472509	3.199044	0.127259
C	-2.966797	3.154953	-0.116815
C	-2.098193	0.282591	3.345862
C	-0.822205	-0.473986	3.105847
C	-1.472569	-3.199006	-0.127211
C	-2.966859	-3.154888	0.116844
C	-2.098134	-0.282638	-3.345865
C	-0.822162	0.473957	-3.105826
C	0.779538	0.766387	-1.423203
C	0.400624	1.900153	-0.648129
C	-4.202792	-0.715548	-2.314135
C	2.089274	-0.484024	1.647853
C	1.348767	-2.714945	0.103254
C	3.102488	-1.316283	1.103955
C	1.348825	2.714950	-0.103234
C	2.726930	2.436078	-0.319969
C	2.089285	0.484006	-1.647827
C	2.726878	-2.436096	0.319979
C	3.740657	-3.252225	-0.235748
C	5.062878	-2.969228	-0.013539
C	5.434453	-1.857137	0.771762
C	4.474190	-1.046381	1.315180
C	3.102516	1.316257	-1.103946
C	4.474212	1.046336	-1.315187
C	5.434492	1.857082	-0.771784
C	5.062941	2.969180	0.013517

C	3.740726	3.252195	0.235742
H	-4.960734	-2.647704	-1.759361
H	-3.292528	-2.677386	-2.358383
H	-4.960718	2.647730	1.759334
H	-3.292524	2.677378	2.358396
H	-4.599052	0.762466	3.332054
H	-4.904809	0.168765	1.686554
H	-1.228988	3.160436	1.192682
H	-1.044691	4.103798	-0.310583
H	-3.152748	3.125709	-1.188735
H	-3.450777	4.038568	0.305111
H	-2.537023	-0.022072	4.300341
H	-1.884645	1.354127	3.379038
H	-0.129096	-0.331237	3.936653
H	-1.034664	-1.536149	2.981544
H	-1.229038	-3.160421	-1.192633
H	-1.044768	-4.103758	0.310651
H	-3.152823	-3.125609	1.188760
H	-3.450845	-4.038510	-0.305062
H	-2.536918	0.021967	-4.300383
H	-1.884577	-1.354174	-3.378969
H	-0.129017	0.331186	-3.936598
H	-1.034632	1.536123	-2.981564
H	-4.599015	-0.762504	-3.332140
H	-4.904823	-0.168743	-1.686671
H	2.353518	0.392163	2.225696
H	1.078206	-3.569215	-0.501296
H	1.078281	3.569228	0.501312
H	2.353514	-0.392190	-2.225664
H	3.456568	-4.109022	-0.833151
H	5.828980	-3.603560	-0.437574
H	6.481402	-1.645392	0.938400
H	4.750760	-0.180461	1.902815
H	4.750763	0.180410	-1.902822
H	6.481436	1.645323	-0.938434
H	5.829057	3.603503	0.437541
H	3.456656	4.108997	0.833146

(e) Na⁺(DN24C8) (closed')

Na	-1.892846	-0.178287	0.014544
O	-3.932205	1.367085	0.129059
O	-3.383905	-1.981793	0.456846
O	-2.567398	-1.050646	-2.077318
O	-1.473417	1.967853	-1.035378
O	-0.006633	-0.112472	-1.565443
O	-2.058205	1.240501	2.078768
O	-0.071742	-0.508737	1.566309
O	-0.734740	-2.622936	0.133129
C	-4.244796	1.853328	1.432854
C	-4.254739	-1.968293	-0.676505
C	-3.482006	-2.132510	-1.969652
C	-0.131563	2.194689	-0.927452
C	0.657709	1.052714	-1.249834
C	-1.461701	-3.156216	1.248943
C	-2.900469	-3.275874	0.814934
C	-1.484696	-1.324758	-2.960397
C	-0.525555	-0.166365	-2.905878
C	-2.384287	3.017572	-0.730992
C	-3.761316	2.397123	-0.840488

C	-1.160292	0.863854	3.112888
C	0.174645	0.556690	2.484261
C	0.983928	-1.263978	1.133595
C	0.606867	-2.407452	0.373649
C	-3.426156	1.095328	2.447002
C	2.012601	1.093209	-1.153008
C	0.462412	3.358500	-0.531054
C	2.662446	2.280018	-0.723791
C	1.555971	-3.221505	-0.160581
C	2.935670	-2.942831	0.028535
C	2.299827	-0.973427	1.345020
C	1.879939	3.422643	-0.417748
C	2.533914	4.603941	0.005884
C	3.897951	4.640584	0.126296
C	4.674505	3.499857	-0.170276
C	4.069295	2.344125	-0.587059
C	3.307854	-1.808778	0.792741
C	4.682029	-1.518362	0.967061
C	5.639493	-2.325126	0.411197
C	5.268476	-3.459276	-0.342699
C	3.945864	-3.761253	-0.529359
H	-5.310136	1.717722	1.629167
H	-4.007884	2.916294	1.505172
H	-4.743750	-0.996140	-0.659743
H	-5.011028	-2.751582	-0.585670
H	-2.927647	-3.074741	-1.977577
H	-4.174632	-2.131544	-2.816427
H	-1.064680	-4.137699	1.515482
H	-1.368238	-2.483685	2.102751
H	-3.504247	-3.679915	1.630348
H	-2.964664	-3.954208	-0.036585
H	-1.850953	-1.451438	-3.983099
H	-0.978682	-2.238241	-2.636534
H	0.297864	-0.322896	-3.604214
H	-1.037047	0.767272	-3.138449
H	-2.190614	3.383272	0.279355
H	-2.269791	3.834058	-1.447804
H	-3.867912	1.922170	-1.813767
H	-4.534167	3.161016	-0.730806
H	-1.532801	-0.032299	3.618476
H	-1.062043	1.670390	3.843960
H	0.578082	1.417953	1.946495
H	0.877286	0.234704	3.254229
H	-3.604208	1.510768	3.442897
H	-3.691796	0.033672	2.447983
H	2.585844	0.203179	-1.379088
H	-0.120847	4.236665	-0.292639
H	1.247553	-4.078321	-0.745505
H	2.600128	-0.086273	1.884771
H	1.940367	5.480413	0.231668
H	4.386818	5.549461	0.448357
H	5.750049	3.545501	-0.072549
H	4.655949	1.465239	-0.823097
H	4.964064	-0.651078	1.550488
H	6.686972	-2.098120	0.552901
H	6.034490	-4.090048	-0.771268
H	3.656631	-4.630243	-1.105954

(f) Na⁺(DN24C8) (open)

Na	0.000001	0.814220	0.000002
O	-0.666227	2.782317	-1.329728
O	0.666229	2.782345	1.329682
O	-0.149010	0.425184	2.382577
O	-2.474922	1.280285	0.059862
O	-1.445514	-1.144406	0.448850
O	0.148994	0.425118	-2.382575
O	1.445517	-1.144416	-0.448822
O	2.474923	1.280282	-0.059874
C	-0.883971	2.507715	-2.707807
C	0.883966	2.507781	2.707770
C	-0.237066	1.608215	3.159222
C	-3.371102	0.242870	0.080994
C	-2.814420	-1.048722	0.301789
C	2.943635	2.507967	0.493915
C	1.746113	3.422294	0.666332
C	-1.075794	-0.578295	2.766425
C	-1.004480	-1.660343	1.718406
C	-2.943633	2.507961	-0.493951
C	-1.746109	3.422280	-0.666388
C	1.075772	-0.578372	-2.766407
C	1.004474	-1.660392	-1.718359
C	2.814423	-1.048729	-0.301770
C	3.371104	0.242868	-0.080994
C	0.237055	1.608134	-3.159241
C	-3.616859	-2.150807	0.318884
C	-4.720558	0.380681	-0.097757
C	-5.017760	-2.036996	0.142356
C	4.720560	0.380683	0.097751
C	5.574475	-0.752402	0.067247
C	3.616865	-2.150812	-0.318856
C	-5.574470	-0.752406	-0.067243
C	-6.973624	-0.630797	-0.244056
C	-1.775793	-1.739485	-0.216761
C	-7.218691	-3.021322	-0.013462
C	-5.869417	-3.167314	0.161818
C	5.017767	-2.036996	-0.142335
C	5.869426	-3.167312	-0.161787
C	7.218700	-3.021316	0.013487
C	7.775801	-1.739476	0.216770
C	6.973629	-0.630789	0.244056
H	-0.889755	3.437818	-3.282782
H	-1.831772	1.985626	-2.852554
H	0.889751	3.437900	3.282719
H	1.831765	1.985692	2.852535
H	-0.124875	1.378274	4.222686
H	-1.207307	2.087695	2.995028
H	3.444897	2.300272	1.440687
H	3.659127	2.986082	-0.179178
H	1.353419	3.708408	-0.305957
H	2.057178	4.320208	1.208846
H	-2.087182	-0.159931	2.814000
H	-0.811510	-0.983732	3.747655
H	0.027044	-1.966467	1.563454
H	-1.609083	-2.518109	2.008542
H	-3.444896	2.300248	-1.440719
H	-3.659124	2.986090	0.179133
H	-1.353412	3.708412	0.305895
H	-2.057173	4.320186	-1.208917

H	2.087160	-0.160010	-2.814007
H	0.811476	-0.983836	-3.747623
H	-0.027047	-1.966518	-1.563388
H	1.609079	-2.518162	-2.008477
H	0.124862	1.378173	-4.222701
H	1.207298	2.087612	-2.995058
H	-3.175806	-3.130132	0.454881
H	-5.167870	1.351193	-0.255074
H	5.167871	1.351198	0.255055
H	3.175816	-3.130140	-0.454838
H	-7.399957	0.351391	-0.401662
H	-8.843426	-1.637697	-0.352193
H	-7.864770	-3.887670	0.003490
H	-5.437591	-4.147193	0.318603
H	5.437602	-4.147194	-0.318561
H	7.864780	-3.887663	-0.003458
H	8.843433	-1.637684	0.352198
H	7.399960	0.351402	0.401650

(g) K⁺(DN24C8) (closed)

K	0.000000	0.000000	2.432295
O	2.612824	0.328017	3.348978
O	-2.612824	-0.328017	3.348978
O	-1.484644	2.240959	3.071901
O	1.801577	1.482288	0.889268
O	-0.792353	1.793579	0.395956
O	1.484644	-2.240959	3.071901
O	0.792353	-1.793579	0.395956
O	-1.801577	-1.482288	0.889268
C	3.413100	-0.833760	3.518468
C	-3.413100	0.833760	3.518468
C	-2.512558	1.946579	4.008574
C	1.457055	1.512437	-0.434416
C	0.065810	1.698781	-0.682740
C	-3.180390	-1.326833	1.208105
C	-3.294367	-1.401947	2.714774
C	-1.893424	3.116483	2.030632
C	-0.833714	3.112657	0.963810
C	3.180390	1.326833	1.208105
C	3.294367	1.401947	2.714774
C	1.893424	-3.116483	2.030632
C	0.833714	-3.112657	0.963810
C	-0.065810	-1.698781	-0.682740
C	-1.457055	-1.512437	-0.434416
C	2.512558	-1.946579	4.008574
C	-0.410551	1.756231	-1.955155
C	2.325529	1.379803	-1.481191
C	0.467235	1.637362	-3.062608
C	-2.325529	-1.379803	-1.481191
C	-1.848729	-1.440275	-2.819116
C	0.410551	-1.756231	-1.955155
C	1.848729	1.440275	-2.819116
C	2.725983	1.314574	-3.922301
C	2.248362	1.396739	-5.204119
C	0.872846	1.601109	-5.443501
C	0.000000	1.712531	-4.394780
C	-0.467235	-1.637362	-3.062608
C	0.000000	-1.712531	-4.394780
C	-0.872846	-1.601109	-5.443501

C	-2.248362	-1.396739	-5.204119
C	-2.725983	-1.314574	-3.922301
H	4.195895	-0.643605	4.259203
H	3.891805	-1.106232	2.573652
H	-4.195895	0.643605	4.259203
H	-3.891805	1.106232	2.573652
H	-3.103500	2.841328	4.223323
H	-2.015738	1.630853	4.924379
H	-3.535646	-0.366645	0.825309
H	-3.761744	-2.132632	0.753182
H	-2.828495	-2.321269	3.065782
H	-4.347823	-1.411484	3.006702
H	-2.018104	4.129830	2.423436
H	-2.839977	2.784921	1.596214
H	-1.086620	3.832997	0.183547
H	0.141632	3.358049	1.386908
H	3.535646	0.366645	0.825309
H	3.761744	2.132632	0.753182
H	2.828495	2.321269	3.065782
H	4.347823	1.411484	3.006702
H	2.018104	-4.129830	2.423436
H	2.839977	-2.784921	1.596214
H	1.086620	-3.832997	0.183547
H	-0.141632	-3.358049	1.386908
H	3.103500	-2.841328	4.223323
H	2.015738	-1.630853	4.924379
H	-1.473505	1.884883	-2.113772
H	3.383711	1.233429	-1.320091
H	-3.383711	-1.233429	-1.320091
H	1.473505	-1.884883	-2.113772
H	3.782481	1.165356	-3.739473
H	2.928877	1.309641	-6.039913
H	0.509773	1.660874	-6.460009
H	-1.059276	1.848481	-4.570618
H	1.059276	-1.848481	-4.570618
H	-0.509773	-1.660874	-6.460009
H	-2.928877	-1.309641	-6.039913
H	-3.782481	-1.165356	-3.739473

(h) $K^+(\text{DN24C8})$ (closed')

K	-2.211911	-0.148879	0.173718
O	-3.493845	2.316470	0.564882
O	-3.223350	-2.759895	-0.115616
O	-2.951317	-1.087255	-2.355599
O	-1.521260	2.060286	-1.429535
O	-0.338301	-0.253128	-1.886245
O	-2.319001	1.059983	2.732465
O	0.082715	0.013094	1.842773
O	-0.636154	-2.381282	0.951071
C	-4.080123	2.388907	1.855962
C	-3.524390	-3.257614	-1.412971
C	-3.953356	-2.088418	-2.272948
C	-0.156943	2.085904	-1.324112
C	0.465811	0.835937	-1.621561
C	-1.069176	-3.669177	0.527144
C	-2.569444	-3.709554	0.715075
C	-1.895089	-1.394377	-3.253839
C	-0.901812	-0.265775	-3.207254
C	-2.272593	3.254475	-1.216444

C	-2.634863	3.400865	0.243371
C	-1.204186	0.942222	3.603505
C	-0.382359	-0.242199	3.176495
C	1.078649	-0.848536	1.431747
C	0.707706	-2.126169	0.924184
C	-3.062267	2.243502	2.967564
C	1.817512	0.701126	-1.568117
C	0.607858	3.158367	-0.960382
C	2.637348	1.800554	-1.207953
C	1.667251	-2.981289	0.458445
C	3.036962	-2.602041	0.485904
C	2.383652	-0.467622	1.471662
C	2.023183	3.038179	-0.895489
C	2.840408	4.131049	-0.520195
C	4.201970	3.994241	-0.459427
C	4.812226	2.760317	-0.772662
C	4.045569	1.686173	-1.139273
C	3.403106	-1.335003	1.003309
C	4.769216	-0.966730	1.035488
C	5.730596	-1.823032	0.569299
C	5.366661	-3.084642	0.049562
C	4.052162	-3.466187	0.009471
H	-4.795887	1.570146	1.900167
H	-4.621490	3.332328	1.976328
H	-4.339511	-3.985200	-1.354297
H	-2.650978	-3.757739	-1.839787
H	-4.226239	-2.443124	-3.271365
H	-4.823198	-1.610992	-1.824890
H	-0.793900	-3.820827	-0.519668
H	-0.594684	-4.442040	1.136906
H	-2.811514	-3.449656	1.744353
H	-2.943209	-4.716893	0.513886
H	-2.286019	-1.499061	-4.270527
H	-1.396681	-2.324224	-2.966159
H	-0.105990	-0.429920	-3.936124
H	-1.398954	0.683241	-3.403562
H	-1.730855	4.123581	-1.587166
H	-3.181894	3.128117	-1.799206
H	-3.152868	4.352518	0.402369
H	-1.732319	3.374554	0.860495
H	-1.540025	0.804594	4.635921
H	-0.595488	1.849330	3.543133
H	0.473749	-0.356057	3.843970
H	-0.975848	-1.158225	3.187938
H	-2.384109	3.101834	2.999574
H	-3.583195	2.189448	3.928835
H	2.258322	-0.265989	-1.775590
H	0.165488	4.111618	-0.709547
H	1.413266	-3.955246	0.066215
H	2.632476	0.518925	1.841772
H	2.374602	5.079666	-0.286192
H	4.816813	4.836993	-0.175373
H	5.888643	2.669473	-0.727620
H	4.503890	0.735697	-1.379668
H	5.038106	0.003083	1.433592
H	6.773171	-1.538990	0.601180
H	6.134396	-3.753343	-0.314026
H	3.774869	-4.435830	-0.383451

(i) K⁺(DN24C8) (open)

K	0.000000	0.000000	0.232599
O	1.383995	0.680146	2.502282
O	-1.383995	-0.680146	2.502282
O	-2.714414	0.635657	0.465702
O	0.076227	2.725553	1.062338
O	-0.981484	2.070800	-1.301373
O	2.714414	-0.635657	0.465702
O	0.981484	-2.070800	-1.301373
O	-0.076227	-2.725553	1.062338
C	2.791562	0.790777	2.350087
C	-2.791562	-0.790777	2.350087
C	-3.282934	0.504239	1.757111
C	0.000000	3.733277	0.137062
C	-0.576845	3.377279	-1.116436
C	-0.737531	-3.034121	2.285593
C	-0.756871	-1.782820	3.136934
C	-3.124622	1.821410	-0.196158
C	-2.391100	1.889997	-1.512081
C	0.737531	3.034121	2.285593
C	0.756871	1.782820	3.136934
C	3.124622	-1.821410	-0.196158
C	2.391100	-1.889997	-1.512081
C	0.576845	-3.377279	-1.116436
C	0.000000	-3.733277	0.137062
C	3.282934	-0.504239	1.757111
C	-0.676788	4.298201	-2.116404
C	0.435977	5.014744	0.342004
C	-0.239600	5.632205	-1.928946
C	-0.435977	-5.014744	0.342004
C	-0.321932	-5.992377	-0.680774
C	0.676788	-4.298201	-2.116404
C	0.321932	5.992377	-0.680774
C	0.762616	7.323219	-0.485178
C	0.650258	8.246596	-1.489395
C	0.094334	7.884618	-2.736159
C	-0.340697	6.605179	-2.951760
C	0.239600	-5.632205	-1.928946
C	0.340697	-6.605179	-2.951760
C	-0.094334	-7.884618	-2.736159
C	-0.650258	-8.246596	-1.489395
C	-0.762616	-7.323219	-0.485178
H	3.264405	0.959857	3.322614
H	3.047587	1.613134	1.677532
H	-3.264405	-0.959857	3.322614
H	-3.047587	-1.613134	1.677532
H	-4.375320	0.489106	1.691322
H	-2.975159	1.345963	2.385940
H	-1.745085	-3.397116	2.072081
H	-0.193365	-3.815339	2.822592
H	0.261378	-1.456177	3.336845
H	-1.254782	-2.010259	4.085191
H	-2.884696	2.697435	0.416199
H	-4.204504	1.798626	-0.375507
H	-2.499027	0.949504	-2.048468
H	-2.784511	2.700968	-2.123557
H	1.745085	3.397116	2.072081
H	0.193365	3.815339	2.822592
H	-0.261378	1.456177	3.336845

H	1.254782	2.010259	4.085191
H	2.884696	-2.697435	0.416199
H	4.204504	-1.798626	-0.375507
H	2.499027	-0.949504	-2.048468
H	2.784511	-2.700968	-2.123557
H	4.375320	-0.489106	1.691322
H	2.975159	-1.345963	2.385940
H	-1.085437	3.999102	-3.073441
H	0.870642	5.316734	1.283081
H	-0.870642	-5.316734	1.283081
H	1.085437	-3.999102	-3.073441
H	1.190394	7.600369	0.469561
H	0.989279	9.260821	-1.331280
H	0.013795	8.624450	-3.519997
H	-0.767604	6.321888	-3.904991
H	0.767604	-6.321888	-3.904991
H	-0.013795	-8.624450	-3.519997
H	-0.989279	-9.260821	-1.331280
H	-1.190394	-7.600369	0.469561

(j) Rb⁺(DN24C8) (closed)

Rb	-2.388770	-0.199259	0.403026
O	-3.040126	-3.071152	0.183512
O	-3.668398	2.502657	0.252953
O	-1.806820	2.174740	2.237395
O	-0.460154	-2.329029	1.217196
O	0.031668	0.021159	2.182932
O	-3.025661	-1.494911	-2.167677
O	-0.418598	-0.524472	-1.781705
O	-1.287878	1.951705	-1.301432
C	-3.287709	-3.662934	-1.084390
C	-3.651801	3.373884	1.378351
C	-3.105349	2.633534	2.574010
C	0.852769	-1.952386	1.181693
C	1.127777	-0.661043	1.733864
C	-1.803507	3.264935	-1.104769
C	-3.305748	3.140281	-0.966742
C	-1.042040	1.771157	3.361689
C	0.278595	1.246371	2.865825
C	-0.760414	-3.655874	0.801393
C	-2.237967	-3.882242	1.032865
C	-1.984471	-1.714395	-3.107987
C	-1.048840	-0.536856	-3.070873
C	0.517997	0.477906	-1.635353
C	0.070308	1.806900	-1.369537
C	-3.886332	-2.610551	-1.993301
C	2.409535	-0.196725	1.783036
C	1.869693	-2.710336	0.677977
C	3.486126	-0.980031	1.285360
C	0.982211	2.811543	-1.196638
C	2.375269	2.536200	-1.266219
C	1.846770	0.193502	-1.696364
C	3.212112	-2.241637	0.711553
C	4.280948	-3.010506	0.195268
C	5.569101	-2.545499	0.262503
C	5.843202	-1.292227	0.848755
C	4.822549	-0.524269	1.344955
C	2.815216	1.212955	-1.514027
C	4.201348	0.940767	-1.574685

C	5.113536	1.947472	-1.403849
C	4.677611	3.267969	-1.161281
C	3.340113	3.556818	-1.091971
H	-3.993641	-4.492517	-0.977736
H	-2.359929	-4.058908	-1.505348
H	-4.663727	3.729984	1.584829
H	-3.010921	4.235437	1.181243
H	-3.064799	3.314588	3.429892
H	-3.749918	1.788476	2.840914
H	-1.370374	3.692807	-0.198436
H	-1.549282	3.892688	-1.962612
H	-3.698136	2.522875	-1.772805
H	-3.767691	4.128528	-1.031410
H	-1.567380	0.992363	3.924028
H	-0.866789	2.625404	4.022700
H	0.730762	1.968279	2.181543
H	0.948086	1.067720	3.710096
H	-0.502413	-3.776598	-0.254054
H	-0.181573	-4.368707	1.394157
H	-2.486759	-3.613506	2.057987
H	-2.476383	-4.938823	0.884164
H	-2.405293	-1.817168	-4.112959
H	-1.424718	-2.620787	-2.863441
H	-0.285099	-0.644040	-3.843809
H	-1.596366	0.394141	-3.221323
H	-4.136288	-3.057528	-2.960222
H	-4.801112	-2.225349	-1.545689
H	2.637093	0.776271	2.192315
H	1.682507	-3.686077	0.254824
H	0.670187	3.829106	-1.012220
H	2.157646	-0.828397	-1.871905
H	4.069483	-3.977102	-0.243983
H	6.381055	-3.143568	-0.127265
H	6.863291	-0.937948	0.902327
H	5.026275	0.445174	1.780914
H	4.527105	-0.077297	-1.746316
H	6.172165	1.733200	-1.451690
H	5.406971	4.055802	-1.032864
H	3.006550	4.570372	-0.909840

(k) Rb⁺(DN24C8) (closed')

Rb	-2.357422	-0.104561	0.196111
O	-3.212134	2.704042	0.595184
O	-3.078307	-2.956355	-0.144413
O	-2.905858	-1.309966	-2.450787
O	-1.364499	2.148565	-1.524300
O	-0.349415	-0.270350	-1.961162
O	-2.137166	1.380416	2.814135
O	0.108832	0.042257	1.897372
O	-0.545274	-2.424016	1.098430
C	-3.706093	2.923721	1.908094
C	-3.225105	-3.508560	-1.446015
C	-3.769990	-2.431910	-2.360056
C	0.000364	2.068992	-1.456966
C	0.525746	0.769853	-1.732959
C	-0.918922	-3.729992	0.672742
C	-2.425286	-3.829057	0.766891
C	-1.826214	-1.487712	-3.356538
C	-0.928897	-0.282538	-3.273826

C	-2.001822	3.407053	-1.309491
C	-2.249028	3.653864	0.162232
C	-1.028534	1.136443	3.666526
C	-0.355339	-0.141078	3.241935
C	1.122152	-0.813822	1.523209
C	0.789238	-2.123601	1.071491
C	-2.665253	2.684383	2.981592
C	1.866090	0.540965	-1.698437
C	0.851302	3.092986	-1.145681
C	2.772069	1.587477	-1.392173
C	1.779329	-2.968728	0.650203
C	3.137376	-2.550006	0.665255
C	2.416094	-0.393349	1.543227
C	2.255653	2.875553	-1.109982
C	3.157242	3.919832	-0.794117
C	4.507058	3.688545	-0.763003
C	5.019908	2.404049	-1.046278
C	4.169846	1.375221	-1.353884
C	3.464186	-1.250388	1.122624
C	4.819083	-0.842934	1.147276
C	5.807580	-1.693550	0.730101
C	5.482682	-2.987680	0.267330
C	4.179436	-3.407103	0.236175
H	-4.532489	2.226546	2.034143
H	-4.095028	3.942544	2.001731
H	-3.928229	-4.346994	-1.417198
H	-2.264869	-3.880515	-1.812625
H	-3.957820	-2.852733	-3.352426
H	-4.712488	-2.063092	-1.958427
H	-0.575713	-3.890403	-0.351976
H	-0.458451	-4.478647	1.322496
H	-2.745338	-3.539164	1.766509
H	-2.735351	-4.862998	0.591616
H	-2.208916	-1.589005	-4.376784
H	-1.249615	-2.381195	-3.102476
H	-0.133448	-0.358419	-4.017963
H	-1.499661	0.632103	-3.432983
H	-1.420684	4.212277	-1.757607
H	-2.957669	3.335382	-1.823041
H	-2.635875	4.669168	0.300976
H	-1.318671	3.544051	0.725659
H	-1.358410	1.053409	4.706814
H	-0.314994	1.961526	3.583436
H	0.494282	-0.339450	3.897810
H	-1.043882	-0.987476	3.281512
H	-1.855873	3.418226	2.917468
H	-3.136717	2.788661	3.964449
H	2.231774	-0.460797	-1.886365
H	0.486134	4.083413	-0.916106
H	1.559857	-3.968383	0.305561
H	2.633548	0.616588	1.867220
H	2.765768	4.906824	-0.583641
H	5.187384	4.494707	-0.525831
H	6.087998	2.237472	-1.023663
H	4.554083	0.386275	-1.567263
H	5.057706	0.152942	1.496968
H	6.841688	-1.379383	0.756023
H	6.271360	-3.651367	-0.058829
H	3.932078	-4.401675	-0.111958

(l) Rb⁺(DN24C8) (open)

Rb	-0.042483	-1.338848	0.016142
O	-1.832049	-2.965871	1.814046
O	1.580028	-3.244073	-1.523258
O	-0.901835	-2.366257	-2.656179
O	-3.056881	-0.856964	0.350791
O	-1.891947	0.174802	-1.796812
O	0.549434	-1.910230	2.975303
O	2.533154	-0.571306	1.470758
O	2.654306	-0.665008	-1.189644
C	-1.592730	-2.929436	3.213175
C	0.780964	-4.030650	-2.396882
C	0.002190	-3.184606	-3.380379
C	-3.385221	0.442377	0.078570
C	-2.741908	0.985343	-1.071960
C	3.472261	-1.844709	-1.186328
C	2.822920	-2.856745	-2.090065
C	-1.592527	-1.465525	-3.508104
C	-2.596689	-0.686111	-2.705255
C	-3.737210	-1.501519	1.421188
C	-3.211197	-2.918479	1.476973
C	1.923181	-1.910947	3.326196
C	2.544865	-0.610921	2.894142
C	3.174595	0.479836	0.872080
C	3.236420	0.409466	-0.550092
C	-0.114615	-3.068375	3.458665
C	-2.947993	2.280687	-1.433508
C	-4.238816	1.215731	0.814425
C	-3.816413	3.113135	-0.681778
C	3.827135	1.404038	-1.266922
C	4.399460	2.526626	-0.616479
C	3.720475	1.548443	1.527310
C	-4.475370	2.568294	0.447628
C	-5.353117	3.391822	1.191671
C	-5.561046	4.695106	0.826799
C	-4.902193	5.237584	-0.297560
C	-4.048196	4.463051	-1.035621
C	4.347710	2.593700	0.797237
C	4.920944	3.709831	1.451651
C	5.516827	4.708866	0.729490
C	5.567752	4.640903	-0.679685
C	5.020175	3.573119	-1.338274
H	-2.114356	-3.760084	3.698665
H	-1.943967	-1.988283	3.645103
H	0.084675	-4.582378	-1.767195
H	1.403811	-4.748903	-2.938166
H	0.670152	-2.555393	-3.977150
H	-0.548439	-3.840887	-4.063036
H	4.465137	-1.594836	-1.565677
H	3.555419	-2.229589	-0.168851
H	3.475196	-3.730123	-2.188160
H	2.676192	-2.410963	-3.076773
H	-2.122232	-2.021132	-4.289044
H	-0.881095	-0.781710	-3.981335
H	-3.204382	-0.073655	-3.374458
H	-3.241156	-1.361099	-2.140148
H	-3.547601	-0.968653	2.355847
H	-4.813128	-1.508567	1.228745

H	-3.307397	-3.374116	0.492898
H	-3.797064	-3.501907	2.192808
H	2.435585	-2.750724	2.845849
H	2.031070	-2.007713	4.411327
H	1.975147	0.230187	3.295031
H	3.574273	-0.560860	3.256087
H	0.057199	-3.172612	4.534775
H	0.266951	-3.960363	2.952093
H	-2.437965	2.668496	-2.305874
H	-4.745826	0.823966	1.684212
H	3.849942	1.327418	-2.346292
H	3.682484	1.628666	2.603776
H	-5.858922	2.976391	2.053615
H	-6.234278	5.315836	1.401371
H	-5.076432	6.267985	-0.573550
H	-3.541115	4.872231	-1.899636
H	4.882353	3.762191	2.531951
H	5.953059	5.556966	1.238507
H	6.042441	5.436672	-1.236214
H	5.056677	3.514537	-2.418251

(m) Cs⁺(DN24C8) (closed)

Cs	-2.398695	-0.191150	0.403925
O	-2.844141	-3.186587	0.153996
O	-3.509692	2.676675	0.178173
O	-1.667249	2.301823	2.185239
O	-0.306283	-2.315044	1.266121
O	0.139428	0.077245	2.196358
O	-2.894499	-1.648707	-2.233574
O	-0.348687	-0.531503	-1.824935
O	-1.155984	1.986636	-1.391626
C	-2.996052	-3.811358	-1.112696
C	-3.443702	3.572055	1.281976
C	-2.944842	2.829627	2.497151
C	0.998030	-1.907636	1.235870
C	1.246147	-0.600215	1.764396
C	-1.620609	3.320937	-1.209440
C	-3.125509	3.265208	-1.059007
C	-0.943302	1.866397	3.324268
C	0.378279	1.314479	2.861178
C	-0.560580	-3.656980	0.866425
C	-2.035821	-3.931613	1.055248
C	-1.840400	-1.789553	-3.174224
C	-0.973562	-0.560763	-3.115847
C	0.609365	0.451535	-1.690663
C	0.197290	1.797388	-1.452826
C	-3.662284	-2.829033	-2.052579
C	2.520903	-0.115043	1.813540
C	2.034631	-2.656147	0.756739
C	3.615606	-0.887695	1.340362
C	1.138142	2.778851	-1.298918
C	2.523026	2.464910	-1.359750
C	1.930717	0.130422	-1.740409
C	3.368349	-2.164764	0.790626
C	4.454304	-2.926400	0.300054
C	5.733894	-2.438582	0.369635
C	5.981298	-1.168733	0.931650
C	4.943389	-0.407864	1.402144
C	2.927419	1.125387	-1.577324

C	4.305783	0.814953	-1.630240
C	5.244258	1.800900	-1.483306
C	4.843866	3.137667	-1.271013
C	3.514550	3.463279	-1.207640
H	-3.624942	-4.702209	-1.016235
H	-2.023447	-4.122149	-1.502763
H	-4.433289	3.992055	1.477045
H	-2.752785	4.389755	1.067814
H	-2.879870	3.524689	3.340334
H	-3.634129	2.023590	2.773760
H	-1.164521	3.743750	-0.312068
H	-1.347153	3.926910	-2.077068
H	-3.551332	2.647303	-1.847571
H	-3.542383	4.271729	-1.146777
H	-1.503289	1.097971	3.867592
H	-0.762838	2.709904	3.997768
H	0.847036	2.021650	2.172968
H	1.032080	1.146664	3.719944
H	-0.267737	-3.789522	-0.178060
H	0.021173	-4.342078	1.488485
H	-2.331014	-3.641017	2.062041
H	-2.224703	-5.002166	0.935782
H	-2.252553	-1.900031	-4.182049
H	-1.228850	-2.665601	-2.943377
H	-0.203345	-0.615403	-3.887989
H	-1.570234	0.341389	-3.256725
H	-3.855119	-3.312869	-3.014854
H	-4.615134	-2.515602	-1.628824
H	2.730349	0.867983	2.207496
H	1.870692	-3.644388	0.354185
H	0.855995	3.808806	-1.137737
H	2.213145	-0.902941	-1.895610
H	4.263030	-3.905479	-0.120487
H	6.559436	-3.030905	0.000109
H	6.994709	-0.795934	0.986394
H	5.126889	0.574195	1.818497
H	4.605015	-0.215414	-1.775427
H	6.296724	1.556934	-1.524141
H	5.593968	3.908596	-1.160584
H	3.207995	4.489107	-1.048019

(n) Cs⁺(DN24C8) (closed')

Cs	-2.412717	-0.055790	0.216696
O	-2.959788	2.947704	0.509498
O	-2.940649	-3.055379	-0.089062
O	-2.830522	-1.488130	-2.463809
O	-1.190874	2.128379	-1.627046
O	-0.304486	-0.364367	-1.976525
O	-1.955763	1.658625	2.796065
O	0.169799	0.124717	1.902702
O	-0.429835	-2.386449	1.184486
C	-3.392829	3.286564	1.818352
C	-3.030533	-3.659885	-1.371974
C	-3.628430	-2.654049	-2.332630
C	0.168093	1.974983	-1.570018
C	0.621938	0.639109	-1.792611
C	-0.763122	-3.713319	0.791107
C	-2.266516	-3.860446	0.867194
C	-1.743267	-1.636632	-3.365182

C	-0.882012	-0.404836	-3.289105
C	-1.747020	3.432518	-1.464406
C	-1.931720	3.781929	-0.003717
C	-0.859617	1.359919	3.646528
C	-0.287094	0.022329	3.257613
C	1.201250	-0.727182	1.573730
C	0.897482	-2.057166	1.161055
C	-2.349991	3.016308	2.882686
C	1.949552	0.343152	-1.761662
C	1.076726	2.965786	-1.317915
C	2.913497	1.353361	-1.517747
C	1.910127	-2.895340	0.779412
C	3.260571	-2.453111	0.803392
C	2.487936	-0.284940	1.602015
C	2.468411	2.678299	-1.291172
C	3.427296	3.688747	-1.040868
C	4.764130	3.389907	-1.021363
C	5.205649	2.068465	-1.249099
C	4.298867	1.071005	-1.490519
C	3.558287	-1.136648	1.230314
C	4.905687	-0.707161	1.271373
C	5.915553	-1.552723	0.897698
C	5.619800	-2.862902	0.461330
C	4.323928	-3.303899	0.415787
H	-4.275330	2.677431	2.005876
H	-3.685326	4.340659	1.859686
H	-3.679249	-4.540507	-1.323587
H	-2.042919	-3.981414	-1.712363
H	-3.782617	-3.125238	-3.308123
H	-4.595054	-2.326463	-1.952962
H	-0.400664	-3.892829	-0.223645
H	-0.290638	-4.430021	1.467902
H	-2.611902	-3.541061	1.849314
H	-2.534900	-4.912407	0.733787
H	-2.119728	-1.757006	-4.385773
H	-1.139555	-2.509726	-3.103804
H	-0.084154	-0.465117	-4.032273
H	-1.476143	0.493427	-3.458173
H	-1.134960	4.174181	-1.976811
H	-2.721828	3.390841	-1.944612
H	-2.226369	4.833567	0.082403
H	-0.998516	3.625104	0.543210
H	-1.182546	1.337138	4.692121
H	-0.086129	2.124568	3.529150
H	0.553505	-0.215990	3.911584
H	-1.034220	-0.770460	3.335445
H	-1.475361	3.660845	2.750797
H	-2.782286	3.233206	3.865334
H	2.260382	-0.683618	-1.908822
H	0.767878	3.984133	-1.132550
H	1.715177	-3.909189	0.463059
H	2.683017	0.738669	1.896060
H	3.090309	4.703582	-0.872678
H	5.488791	4.170621	-0.835751
H	6.263869	1.847067	-1.233284
H	4.628479	0.053479	-1.656276
H	5.121693	0.302095	1.596367
H	6.943935	-1.221369	0.935724
H	6.424870	-3.522262	0.167951

H	4.099088	-4.311134	0.089389
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(o) Cs⁺(DN24C8) (open)

Cs	-0.012612	-1.108745	0.010611
O	-1.704293	-2.802715	2.003888
O	1.582718	-3.045365	-1.721309
O	-1.029655	-2.282518	-2.684603
O	-3.142975	-0.830361	0.502061
O	-2.196298	0.175826	-1.773776
O	0.794417	-1.786745	3.005142
O	2.787302	-0.534990	1.388217
O	2.743769	-0.498825	-1.284767
C	-1.392137	-2.675070	3.383216
C	0.763489	-3.844970	-2.563306
C	-0.111320	-3.016293	-3.478082
C	-3.581013	0.426843	0.189438
C	-3.057975	0.953845	-1.028042
C	3.519343	-1.700264	-1.407861
C	2.791798	-2.631547	-2.338703
C	-1.877607	-1.468432	-3.478852
C	-2.882907	-0.778454	-2.598462
C	-3.710195	-1.460981	1.644656
C	-3.097717	-2.840934	1.733877
C	2.188540	-1.892558	3.243138
C	2.870391	-0.624307	2.807057
C	3.433793	0.517319	0.797408
C	3.405489	0.517493	-0.628101
C	0.087391	-2.880234	3.571134
C	-3.385802	2.210494	-1.434752
C	-4.438721	1.176667	0.945452
C	-4.262523	3.017333	-0.665454
C	3.991980	1.524289	-1.331809
C	4.649769	2.589806	-0.666964
C	4.064984	1.530304	1.465522
C	-4.800569	2.487436	0.532735
C	-5.685503	3.284159	1.297260
C	-6.015504	4.547701	0.885736
C	-5.477213	5.075445	-0.307772
C	-4.618965	4.326259	-1.066711
C	4.688807	2.586387	0.748504
C	5.347626	3.644708	1.418254
C	5.938331	4.655734	0.708659
C	5.898335	4.658216	-0.702563
C	5.267038	3.647237	-1.375697
H	-1.928058	-3.439231	3.954831
H	-1.674248	-1.687970	3.760226
H	0.130157	-4.440265	-1.907396
H	1.381677	-4.523319	-3.158802
H	0.487739	-2.327639	-4.082906
H	-0.652928	-3.684529	-4.156635
H	4.497607	-1.453734	-1.825578
H	3.645121	-2.156870	-0.424897
H	3.422112	-3.503248	-2.541700
H	2.589840	-2.113057	-3.279638
H	-2.414382	-2.087091	-4.205860
H	-1.283635	-0.724714	-4.019255
H	-3.610070	-0.251341	-3.219557
H	-3.398501	-1.502383	-1.965550
H	-3.495614	-0.872269	2.539820

H	-4.793695	-1.541631	1.525092
H	-3.214746	-3.345063	0.776047
H	-3.616139	-3.422434	2.501641
H	2.601161	-2.749243	2.700816
H	2.373108	-2.033384	4.313157
H	2.380374	0.238226	3.263929
H	3.918901	-0.652163	3.112615
H	0.303032	-2.943402	4.642687
H	0.394108	-3.815757	3.093149
H	-2.965698	2.587170	-2.358460
H	-4.855681	0.797112	1.866837
H	3.944629	1.501155	-2.412909
H	4.100128	1.557319	2.544581
H	-6.098982	2.880004	2.212140
H	-6.693216	5.148231	1.476273
H	-5.747386	6.074322	-0.620013
H	-4.203979	4.724107	-1.983523
H	5.378771	3.643195	2.500077
H	6.440272	5.459266	1.229266
H	6.369881	5.462745	-1.249067
H	5.233504	3.642613	-2.457355