

Theoretical study of small sodium-potassium alloy clusters through genetic algorithm and quantum chemical calculations

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Supplementary Information

Part I

Structures obtained at the GA/Gupta level

Na2
energy = -0.5751751993 eV

Na	-1.593442	-0.147552	0.482175
Na	1.593442	0.147552	-0.482175

Na3
energy = -1.159436004 eV

Na	0.949385	1.736597	-0.371319
Na	1.000455	-1.742618	-0.131740
Na	-1.949840	0.006020	0.503059

Na4
energy = -1.837674540 eV

Na	-1.668002	-0.267329	1.390329
Na	-0.124196	1.983321	-0.915273
Na	-0.098547	-1.530654	-1.560159
Na	1.890745	-0.185338	1.085102

Na5
energy = -2.512459489 eV

Na	-0.300512	1.002858	-1.843453
Na	-2.288601	-1.651780	-0.525509
Na	1.227760	-1.726443	0.079652
Na	2.288600	1.651781	0.525510
Na	-0.927247	0.723584	1.763799

Na6
energy = -3.267639497 eV

Na	-1.949835	1.641088	0.000070
Na	-1.641081	-1.949831	0.004124
Na	-0.002710	-0.003113	-2.548530
Na	0.002711	0.003113	2.548529
Na	1.641082	1.949829	-0.004124
Na	1.949833	-1.641086	-0.000069

Na7
energy = -3.979762732 eV

Na	-1.132911	0.505999	-2.777590
Na	2.099685	1.497843	-1.613140
Na	0.758682	-1.737752	-0.626027
Na	-2.799878	-1.185090	-0.103490
Na	-0.758678	1.737754	0.626028
Na	2.430600	0.419701	1.780603
Na	-0.597500	-1.238454	2.713617

Na8
energy = -4.717738626 eV

Na	-2.209646	0.007506	1.066511
Na	-2.032088	-1.416929	-2.239079
Na	-0.673386	-3.217244	0.588604
Na	-0.519075	1.778595	-1.608506
Na	-0.078932	2.798700	1.819793
Na	1.237200	-0.548529	2.046593
Na	1.491526	-1.237571	-1.504617
Na	2.784403	1.835472	-0.169300

Na9
energy = -5.468013517 eV

Na	0.088405	0.663840	-2.669437
Na	-0.570351	-2.834936	-2.118390
Na	2.663566	2.282437	-0.738692
Na	2.337205	-1.304081	-0.641342
Na	-2.667669	-0.338491	-0.586052
Na	-0.793941	2.626528	0.213333
Na	-0.418864	-2.306407	1.442055
Na	1.454859	0.658602	2.241442
Na	-2.093209	0.552507	2.857083

Na10
energy = -6.249660636 eV

Na	-2.690325	-0.234077	-0.936569
Na	-1.291055	-1.222106	2.238157
Na	-1.248745	2.246929	1.249654
Na	-0.673803	-3.268422	-0.720207
Na	-0.604542	2.412312	-2.338929
Na	-0.387650	-1.025708	-3.616239
Na	1.177652	-0.178051	-0.574461
Na	1.686804	0.794355	2.859901
Na	1.980039	-2.697538	1.755652
Na	2.051625	3.172308	0.083041

Na11
energy = -7.045905955 eV

Na	-0.486813	1.879903	-2.631943
Na	-0.009714	-1.730840	-2.478756
Na	2.890524	0.466628	-2.029606
Na	-2.894671	-0.197195	-0.849718
Na	1.734866	3.491406	-0.214558
Na	2.475832	-2.560293	0.085624
Na	0.507701	0.337033	0.581844
Na	-1.840847	2.981813	0.642056
Na	-1.150868	-2.967062	0.755132
Na	-2.255593	-0.045122	2.757259
Na	1.029583	-1.656272	3.382665

Na12
energy = -7.929993175 eV

Na	-2.183405	0.109450	-2.952776
Na	0.937202	2.121900	-2.849089
Na	1.127584	-1.604004	-2.804129
Na	-1.706733	-2.867777	-0.755155
Na	3.347975	0.391984	-0.587184
Na	-0.196239	0.308500	-0.081195
Na	-3.643878	0.079295	0.462615
Na	1.405365	3.335531	0.630412
Na	1.690214	-2.656940	0.699296
Na	-1.425905	2.073118	2.677158
Na	-1.238085	-1.652852	2.728111
Na	1.885905	0.361794	2.831936

Na13
energy = -8.886758701 eV

Na	-0.267423	1.255968	-3.308950
Na	-0.011896	-2.401757	-2.613340
Na	2.922647	-0.177356	-2.006191

Na	-3.095270	-0.530781	-1.653980
Na	1.652907	3.068383	-0.671604
Na	-2.066371	2.849947	-0.453923
Na	0.000000	0.000001	0.000001
Na	2.066371	-2.849947	0.453923
Na	-1.652908	-3.068384	0.671604
Na	3.095269	0.530781	1.653980
Na	-2.922646	0.177356	2.006191
Na	0.011896	2.401756	2.613339
Na	0.267423	-1.255968	3.308949

Na14
energy = -9.601875085 eV

Na	-3.339916	0.712211	-1.312202
Na	-2.944250	-2.364217	0.715497
Na	-2.433026	0.972105	2.327942
Na	-1.551804	-2.202217	-2.740863
Na	-0.847758	3.159814	-0.193472
Na	-0.175558	1.234694	-3.275466
Na	-0.154985	-1.914837	3.113470
Na	-0.147395	-0.302638	-0.073563
Na	0.410982	-3.821138	-0.013538
Na	1.214070	1.459148	2.671582
Na	2.104596	-1.651963	-2.495164
Na	2.181751	4.479605	1.088922
Na	2.676845	1.629309	-0.959268
Na	3.006449	-1.389878	1.146123

Na15
energy = -10.43702950 eV

Na	-1.841313	0.102071	-3.347856
Na	1.311194	1.540553	-3.242929
Na	1.100875	-2.244159	-2.310322
Na	-1.427747	3.234858	-1.451313
Na	-2.632002	-2.499629	-1.197375
Na	3.673065	0.377318	-0.987492
Na	-3.704284	0.902260	-0.270264
Na	1.755992	3.393798	-0.088561
Na	-0.000001	0.000007	0.000004
Na	-0.270047	-3.662876	1.057965
Na	2.882473	-2.224409	1.162966
Na	-2.797100	-1.271458	2.273470
Na	-1.100894	2.244151	2.310333
Na	2.663140	1.220098	2.455187
Na	0.386649	-1.112583	3.636188

K2
energy = -0.4918877380 eV

K	-0.277332	-1.087272	-1.739193
K	0.277332	1.087272	1.739193

K3
energy = -0.9923030375 eV

K	-1.132554	1.858161	-1.198908
K	-0.729968	-2.345623	-0.371510
K	1.862523	0.487462	1.570418

K4
energy = -1.573476151 eV

K	-2.246573	-0.596154	-1.361850
K	1.676757	1.380193	-1.593952
K	1.194638	-2.277289	0.802449

K	-0.624822	1.493250	2.153353
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K5
energy = -2.148114420 eV

K	1.287044	-0.157063	-2.255259
K	-0.909999	-3.416714	-0.281376
K	-2.514104	0.668030	0.019066
K	0.909999	3.416715	0.281371
K	1.227059	-0.510967	2.236199

K6
energy = -2.789337011 eV

K	-3.021151	-0.055127	-0.842403
K	-0.829867	-0.380617	3.001086
K	-0.154953	3.113222	0.351991
K	0.154955	-3.113222	-0.351991
K	0.829865	0.380614	-3.001087
K	3.021151	0.055131	0.842402

K7
energy = -3.394283857 eV

K	0.321467	-0.584552	-3.696347
K	0.230404	3.347110	-1.688725
K	-0.031722	-3.708392	-0.595743
K	-2.418355	0.055887	-0.219160
K	2.418345	-0.055895	0.219162
K	-0.179085	2.653188	2.652652
K	-0.341055	-1.707347	3.328160

K8
energy = -4.015251062 eV

K	-3.922285	-0.686165	1.060445
K	-1.537628	2.316998	-1.162044
K	-0.996678	-2.026193	-1.996097
K	-0.606900	-3.434354	2.194669
K	-0.202421	0.935291	2.857888
K	1.956569	0.911746	-3.510036
K	2.572623	3.208786	0.254929
K	2.736720	-1.226109	0.300245

K9
energy = -4.645728349 eV

K	-3.113304	-1.229628	-0.523117
K	-3.097425	3.148252	0.218595
K	-1.203651	0.394698	3.142226
K	-0.632435	-3.869627	2.044342
K	-0.588833	1.427170	-3.015717
K	0.837651	-2.634048	-1.959182
K	1.320823	3.051512	0.649632
K	2.747303	-1.009714	1.706173
K	3.729871	0.721386	-2.262952

K10
energy = -5.311650905 eV

K	-0.694561	2.004279	-2.800923
K	-0.062340	-2.390161	-2.574486
K	3.201052	0.388643	-1.395281
K	-3.977479	-0.635531	-1.228200

K	-3.129284	3.398394	0.651838
K	1.371049	3.918775	0.704453
K	-2.056591	-4.057518	1.036037
K	2.407235	-3.283463	1.075565
K	-0.539412	-0.000609	1.494249
K	3.480331	0.657189	3.036748

K11
energy = -5.982391874 eV

K	1.220795	-1.121966	-4.065594
K	-3.094086	0.340455	-3.694835
K	0.261135	3.084352	-2.570604
K	3.573476	0.720714	-0.692159
K	2.433218	-3.630789	-0.418337
K	-0.769550	-0.679398	-0.211518
K	-3.389768	2.786303	0.155438
K	0.760338	3.105347	1.883288
K	-1.012784	-3.966189	2.566095
K	2.194568	-0.916344	3.245548
K	-2.177343	0.277514	3.802680

K12
energy = -6.728078751 eV

K	-0.766555	-1.477693	-3.595203
K	2.762343	1.312792	-2.892197
K	-1.519229	2.909408	-2.635528
K	2.798536	-2.922983	-1.158957
K	-4.129213	-0.339591	-0.743667
K	-1.460667	-3.944210	0.168924
K	0.090957	0.175332	0.426577
K	1.599620	4.215789	0.459478
K	4.277056	0.599196	1.374975
K	-2.673776	3.191180	1.791697
K	1.658389	-2.660553	3.273202
K	-2.637462	-1.058666	3.530698

K13
energy = -7.539674980 eV

K	-4.334559	0.325354	0.442673
K	-2.429717	-2.223515	-2.871013
K	-2.101202	2.356379	-3.020374
K	-2.079351	-3.529507	1.519578
K	-1.547809	3.880911	1.277905
K	-1.534301	0.243236	4.083743
K	0.000000	0.000000	0.000000
K	1.534301	-0.243236	-4.083743
K	1.547809	-3.880911	-1.277905
K	2.079351	3.529506	-1.519577
K	2.101203	-2.356379	3.020374
K	2.429717	2.223515	2.871013
K	4.334559	-0.325354	-0.442673

K14
energy = -8.136542191 eV

K	-4.475840	-0.418217	0.218544
K	-2.841302	3.530006	-1.396283
K	-2.610001	-0.279644	-3.948846
K	-2.028811	2.362977	2.982297
K	-1.653939	-3.811249	-1.154515
K	-1.426390	-2.154692	3.086652
K	-0.168538	0.219701	-0.343184
K	0.943406	2.625945	-3.833802
K	1.286556	4.293776	0.405119
K	1.661670	-1.884243	-3.734211
K	2.272939	0.870290	3.206405
K	2.421561	-3.156621	4.930798

K	2.513723	-3.095864	0.549087
K	4.104968	0.897837	-0.968063

K15
energy = -8.826129514 eV

K	-2.018515	0.436569	-4.234836
K	2.477611	-0.100895	-4.006325
K	-0.002421	-3.483093	-3.172800
K	0.338565	3.728841	-2.860133
K	-3.957018	-2.129338	-1.416526
K	4.080028	2.219244	-0.791686
K	-3.393988	2.466883	-0.088592
K	-0.000001	0.000000	0.000000
K	3.393984	-2.466867	0.088602
K	-0.880031	-4.545145	0.875236
K	0.756974	4.455177	1.332960
K	-3.538534	-1.402930	2.776550
K	3.202441	1.157229	3.256347
K	0.722414	-2.224989	4.089841
K	-1.181511	1.889313	4.151362

Na1K1
energy = -0.5320626040 eV

Na	1.793017	0.476248	-0.230959
K	-1.793017	-0.476248	0.230959

Na1K2
energy = -1.046777485 eV

Na	0.997988	-1.865265	0.388617
K	-1.534017	0.030714	-1.865303
K	0.536029	1.834551	1.476686

Na1K3
energy = -1.638358942 eV

K	-1.448251	1.682035	-1.465214
K	-1.439634	-2.053236	0.886115
K	2.202204	-0.790791	-1.264306
Na	0.685681	1.161991	1.843405

Na1K4
energy = -2.225985157 eV

K	-2.268037	0.856514	0.909614
K	-0.778547	1.053462	-3.241784
K	0.284057	-2.453115	-0.778809
K	1.121116	-0.777781	3.219198
Na	1.641410	1.320920	-0.108218

Na1K5
energy = -2.869413144 eV

K	-0.167143	-2.213185	-2.264178
K	-2.995977	0.841667	-0.606924
K	3.059594	-0.698382	0.451402
K	-0.858047	-1.932462	2.097515
K	0.230770	2.356467	2.108659
Na	0.730802	1.645895	-1.786474

Na1K6

energy = -3.493872818 eV

K	-1.172819	-0.128594	-3.541708
K	0.503994	3.377164	-1.508801
K	-1.396308	-3.403671	-0.633312
K	2.229505	-0.705213	-0.622811
K	1.316818	2.268775	2.656008
K	0.142394	-1.922018	3.197078
Na	-1.623584	0.513557	0.453545

Na1K7
energy = -4.128801269 eV

K	-1.966825	-2.315928	-2.622885
K	-2.566146	1.895245	-0.930305
K	1.504135	3.864796	-0.465584
K	4.095325	0.288779	0.748830
K	1.030066	-3.067766	0.755172
K	-3.152627	-1.752421	1.566441
K	0.122606	0.963361	2.575112
Na	0.933466	0.123934	-1.626782

Na1K8
energy = -4.819281722 eV

K	-0.981648	1.223895	-3.518635
K	2.568153	-1.603186	-2.382584
K	-1.852073	-2.971368	-1.607164
K	-0.104468	3.842569	0.257139
K	-3.741880	0.879294	0.259453
K	3.445308	1.015499	1.393185
K	1.278172	-3.118707	1.866026
K	-0.611593	0.731985	3.732597
Na	0.000029	0.000019	-0.000017

Na1K9
energy = -5.563842455 eV

K	-3.237001	0.825337	-2.018982
K	-2.523849	2.154691	2.241734
K	-1.948930	-2.323257	2.457575
K	-1.311009	-3.262334	-1.917391
K	0.242359	3.780206	-0.941833
K	1.062601	0.117332	-3.754006
K	1.530461	0.631546	3.534757
K	2.350553	-3.031236	0.722397
K	3.834814	1.107701	-0.324261
Na	0.000001	0.000014	0.000009

Na1K10
energy = -6.276497763 eV

K	-3.794866	-0.803018	-0.760832
K	-3.049294	1.850397	2.660864
K	-1.405072	3.543793	-1.045003
K	-1.077496	-2.037193	3.211473
K	-0.680101	0.119470	-3.891969
K	-0.448502	-3.826871	-0.882193
K	1.312230	2.309571	2.927211
K	2.931108	2.320277	-1.284217
K	3.049283	-1.850493	-2.660917
K	3.162752	-1.625953	1.725563
Na	-0.000043	0.000021	0.000021

Na1K11
energy = -6.956817740 eV

Na	0.139393	-0.205971	0.125318
K	-4.002056	-0.833193	-0.378140

K	-2.397736	2.071082	2.610592
K	-1.963137	2.900882	-1.765131
K	-1.761399	-2.329641	3.209394
K	-1.152578	-0.994670	-3.812569
K	-1.013950	-4.169394	-0.645150
K	1.443249	3.704504	1.023264
K	1.506549	0.393306	4.050200
K	2.212779	1.809830	-2.946489
K	2.715542	-2.583365	-2.186649
K	4.273345	0.236629	0.715359

Na1K12
energy = -7.776208908 eV

Na	0.000003	0.000013	0.000002
K	-3.631298	-1.457355	-1.641989
K	-3.495900	0.546093	2.342375
K	-2.766560	2.911344	-1.369895
K	-1.638288	-3.474525	1.802764
K	-0.458198	0.352514	-4.203833
K	-0.239110	3.594153	2.243015
K	0.239111	-3.594169	-2.243015
K	0.458196	-0.352513	4.203842
K	1.638281	3.474516	-1.802771
K	2.766567	-2.911331	1.369907
K	3.495890	-0.546103	-2.342379
K	3.631305	1.457363	1.641977

Na1K13
energy = -8.366750660 eV

Na	0.012197	-0.403032	0.222186
K	1.071076	1.371425	-3.464279
K	-2.353237	-1.430150	-3.152580
K	-0.168547	5.567755	-3.069296
K	1.853496	-2.912988	-2.691924
K	-2.701858	2.521975	-1.169937
K	4.151371	0.239360	-0.480614
K	-1.346106	-4.425868	0.005867
K	1.404849	3.576115	0.516888
K	-4.133393	-1.087274	0.948765
K	2.670831	-3.394888	1.655948
K	-1.824416	2.061697	3.153301
K	2.383242	0.585378	3.625592
K	-1.019504	-2.269504	3.900082

Na1K14
energy = -9.037140847 eV

Na	-0.323889	0.110997	-0.736735
K	-4.255812	-0.451930	0.841470
K	-3.419635	-0.800724	-3.518923
K	-3.185170	3.176318	-1.513700
K	-1.807133	-3.897444	-0.754102
K	-1.409176	2.565594	2.520362
K	-0.686967	-1.863225	2.969168
K	-0.124644	2.015352	-4.543234
K	0.732105	-2.335642	-4.066262
K	1.009591	0.966230	5.904404
K	1.111999	4.135649	-0.827206
K	2.504149	-2.940826	-0.029600
K	2.818485	1.132748	1.879441
K	3.475438	-2.503223	4.297676
K	3.560661	0.690128	-2.422758

Na2K1
energy = -1.102535403 eV

Na	0.445326	-0.249814	-2.026969
Na	1.530458	0.982904	1.030013
K	-1.975784	-0.733089	0.996956

Na2K2
energy = -1.704046020 eV

Na	-1.646634	-0.893299	-1.263604
Na	1.136200	1.301163	-1.456748
K	-1.058094	1.505747	1.862934
K	1.568528	-1.913610	0.857418

Na2K3
energy = -2.303951461 eV

K	-1.691326	2.831739	-1.001813
K	-0.346669	0.479905	2.504129
K	1.750319	-2.913405	0.575682
Na	-1.410834	-1.140036	-1.073906
Na	1.698511	0.741797	-1.004093

Na2K4
energy = -2.953233109 eV

K	-2.585337	-1.815708	0.693403
K	-1.918021	2.570015	-0.421678
K	1.918020	-2.570013	0.421669
K	2.585340	1.815699	-0.693392
Na	-0.223553	-0.532282	-2.227337
Na	0.223551	0.532289	2.227334

Na2K5
energy = -3.586828598 eV

K	-2.178299	0.159604	-2.980143
K	-1.650055	-3.283379	-0.385325
K	0.303796	3.382014	-1.456513
K	1.158482	-2.188827	2.742024
K	2.366073	1.930593	2.079959
Na	-1.385872	0.573984	1.043728
Na	1.385876	-0.573989	-1.043729

Na2K6
energy = -4.241203149 eV

K	-2.755779	0.762056	-1.705026
K	-2.408076	1.408546	2.727111
K	-0.401069	-2.863461	-2.941653
K	-0.015776	3.901161	-0.025410
K	2.038661	0.808877	2.504336
K	3.000215	-2.830241	0.044584
Na	-0.745678	-1.652686	0.867702
Na	1.287502	0.465748	-1.471644

Na2K7
energy = -4.897925600 eV

K	-2.794763	1.821498	-2.854159
K	-1.035996	3.457177	1.100983
K	-0.899915	-2.393493	-2.872207
K	-0.886771	0.185851	4.098803
K	0.718172	-2.865457	1.291759
K	2.894831	1.022397	1.931080
K	3.590709	-1.701854	-1.818209
Na	-2.295111	-0.397842	0.419443
Na	0.708843	0.871723	-1.297493

Na2K8
energy = -5.647370008 eV

K	-3.460463	0.083210	-1.648949
K	-2.035243	-1.580201	2.839276
K	-0.903817	-3.728382	-1.094770
K	0.169948	3.510917	-1.531440
K	0.527484	-0.423897	-3.931690
K	1.595168	1.847493	2.956856
K	2.377688	-2.583188	1.894690
K	3.808948	0.721324	-0.942214
Na	-2.173772	2.250077	1.524183
Na	0.094059	-0.097352	-0.065942

Na2K9
energy = -6.369639067 eV

K	-1.226255	0.271021	-3.776270
K	1.682782	-2.803240	-2.199482
K	2.549339	2.121894	-2.127474
K	-2.436798	-3.123852	-0.375788
K	-1.222505	3.777240	-0.274733
K	4.230444	-0.755299	0.751967
K	0.821402	-2.723888	2.726437
K	1.687982	2.201482	2.798578
K	-2.433030	0.382296	3.125986
Na	-3.657441	0.653061	-0.649959
Na	0.004081	-0.000714	0.000738

Na2K10
energy = -7.058400739 eV

K	-1.563904	-0.823918	-3.906461
K	1.308340	2.612432	-2.939926
K	2.605794	-1.803127	-2.464392
K	-2.864048	2.932315	-1.557738
K	-0.944202	-3.926578	-0.517482
K	-4.267413	-0.991192	-0.287659
K	3.693560	1.389403	0.525758
K	-0.209499	3.258262	1.972927
K	-1.688575	-1.091476	3.254235
K	2.173271	0.534989	4.568281
Na	-0.216388	0.055839	-0.239075
Na	1.973064	-2.146948	1.591533

Na2K11
energy = -7.875649615 eV

Na	-0.038534	0.008777	-0.056499
Na	1.983818	-0.451420	2.907925
K	-2.363872	0.537943	-3.465006
K	1.241814	-2.136414	-3.417720
K	1.753464	2.285679	-3.080297
K	-2.403095	-3.283578	-1.109217
K	-1.575218	3.871532	-0.563210
K	4.201253	-0.446907	-0.513852
K	-4.144123	0.429512	0.654971
K	1.654245	-3.859561	0.693967
K	2.475074	3.234555	1.235260
K	-1.646062	-2.287262	3.189565
K	-1.138763	2.097145	3.524114

Na2K12
energy = -8.500619365 eV

Na	-0.418663	0.012508	-0.319251
Na	2.313621	-1.467987	1.420791
K	-1.034182	-1.689064	-4.087120

K	0.617994	2.414322	-3.586310
K	3.129558	-1.155602	-2.488475
K	-3.638535	1.571725	-2.415269
K	0.406527	-4.246349	-0.729923
K	-3.713171	-2.543676	-0.607499
K	3.099087	2.425126	0.106028
K	-1.029446	4.114007	0.217885
K	-3.718091	1.031018	2.045747
K	-1.168452	-2.526745	3.093994
K	0.420578	1.570569	3.585155
K	4.733176	0.490148	3.764249

Na2K13
energy = -9.191632092 eV

Na	-0.556231	0.070591	-0.683739
Na	0.859239	-1.064043	2.367330
K	-4.116003	2.270064	-0.261625
K	-4.082519	-1.957731	-1.618758
K	-3.106671	-1.041926	2.657358
K	-2.319387	1.300750	-4.232783
K	-0.846760	2.757340	2.651358
K	-0.729783	-4.135561	0.404195
K	-0.317818	-2.673386	-3.862015
K	-0.193509	4.159200	-1.477308
K	2.148292	1.111268	-3.697126
K	2.401540	1.310498	5.170907
K	3.021735	-2.277601	-1.015616
K	3.094844	1.907141	0.646355
K	4.743031	-1.736605	2.951467

Na3K1
energy = -1.770495675 eV

Na	-1.770042	-1.260622	-0.489740
Na	-0.444417	2.030008	-0.802262
Na	0.021835	0.201883	2.218294
K	2.192624	-0.971269	-0.926292

Na3K2
energy = -2.382013892 eV

Na	-2.060144	-0.121523	-0.393043
Na	1.013373	-1.650796	0.813261
Na	1.046773	1.772322	-0.420218
K	-0.664933	1.135814	3.134082
K	0.664930	-1.135817	-3.134083

Na3K3
energy = -3.029575025 eV

Na	2.229080	-0.916589	-0.292417
Na	1.055096	2.446340	-0.281407
Na	-2.172656	1.047410	0.277363
K	-0.424502	-0.036245	-3.154516
K	-1.214778	-2.816546	0.324002
K	0.527759	0.275631	3.126975

Na3K4
energy = -3.667673104 eV

K	-1.519092	-1.708504	-2.901553
K	-0.754486	0.708890	3.545972
K	2.325271	0.365502	-2.762282
K	2.807881	1.891355	1.307358
Na	-2.809960	-1.235432	0.796440

Na	-0.859327	1.569092	-0.486393
Na	0.809713	-1.590903	0.500457

Na3K5
energy = -4.329252047 eV

K	-2.576736	-1.851641	-0.689762
K	-1.759976	1.868051	-3.192731
K	-1.145651	-1.173045	3.531487
K	1.326556	-3.580905	0.759856
K	2.038586	3.328104	-1.072902
Na	-1.095927	1.617052	0.725303
Na	1.077865	-0.500133	-1.711739
Na	2.135282	0.292518	1.650488

Na3K6
energy = -5.007076813 eV

K	-0.836505	-1.549116	-3.985066
K	2.392710	1.425988	-2.411452
K	-2.716084	-2.685028	0.113125
K	0.745426	3.259108	1.547974
K	3.832265	0.045709	1.573202
K	-3.447852	1.356826	2.291616
Na	-1.189559	0.855655	-0.891055
Na	1.240587	-2.056540	-0.635365
Na	-0.020988	-0.652602	2.397022

Na3K7
energy = -5.717855025 eV

K	-2.375612	-2.775682	-1.042721
K	-2.049630	-0.235817	3.190410
K	-0.745165	0.786414	-3.746048
K	-0.369496	3.713297	1.132063
K	2.262828	-2.424820	-2.050998
K	2.638525	0.502090	2.827172
K	3.076753	2.093797	-1.493244
Na	-3.220902	1.223224	-0.485884
Na	0.096302	0.065536	-0.046724
Na	0.686396	-2.948039	1.715975

Na3K8
energy = -6.460758579 eV

K	-1.426865	-1.249286	-3.472613
K	2.145669	2.083785	-2.590281
K	-2.226167	2.823344	-1.651802
K	0.119649	-3.933940	0.407150
K	-3.658783	-1.431888	0.467695
K	3.692163	-0.600657	1.289455
K	1.393427	3.281973	1.715397
K	-0.039068	-0.973252	3.834954
Na	2.317344	-1.892619	-2.233269
Na	0.000002	-0.000020	-0.000003
Na	-2.317370	1.892562	2.233318

Na3K9
energy = -7.163203889 eV

K	1.457454	0.956146	-3.695073
K	-2.018441	-1.788382	-3.446280
K	-2.626500	2.576078	-2.162993
K	1.505061	-3.285821	-1.210915
K	1.210249	3.803592	-0.092596
K	-4.257319	-0.986516	0.227249
K	-2.300079	2.301871	2.470424
K	3.497802	-2.466211	2.670027
K	-0.938950	-2.410572	2.799182
Na	3.323931	0.297634	-0.216128

Na	-0.307294	0.034885	-0.194888
Na	1.454085	0.967295	2.851991

Na3K10
energy = -7.976477243 eV

K	-3.442372	-0.504841	-2.408044
K	-3.400039	-1.691781	1.865804
K	-0.878533	-3.961766	-1.091573
K	-0.864486	3.100358	-2.809044
K	-0.796812	1.203573	4.020791
K	0.702684	-0.942144	-4.022266
K	0.771732	-2.877628	2.946829
K	3.308318	1.929383	-1.798891
K	3.348617	-2.437521	-0.710130
K	3.350665	0.742439	2.474943
Na	-2.785195	2.142884	0.622713
Na	0.032968	-0.085412	-0.024037
Na	0.652453	3.382455	0.932905

Na3K11
energy = -8.631936599 eV

Na	-3.081597	0.545323	0.442569
Na	-0.100877	1.099120	2.961633
Na	0.353068	-0.139281	-0.387155
K	-3.788651	1.363821	4.183159
K	-2.753569	-2.702816	-1.834104
K	-2.285500	1.532383	-3.326109
K	-1.681725	-2.585671	2.558358
K	-0.987479	3.936754	0.302996
K	0.877835	-1.530928	-4.214707
K	1.238818	-4.157566	-0.551858
K	1.976571	2.665796	-2.924854
K	2.742666	-1.681648	2.810874
K	3.217592	2.554848	1.324682
K	4.272847	-0.900135	-1.345484

Na3K12
energy = -9.323776487 eV

Na	-2.121640	-2.211406	0.709262
Na	-0.406404	-1.125561	-2.450939
Na	0.021745	0.709813	0.551917
K	-3.836700	0.610795	-1.607073
K	-3.547179	0.846741	2.877512
K	-2.071794	4.249670	0.425858
K	-1.713968	-4.835604	-2.220271
K	-0.131583	2.718425	-3.276272
K	-0.022127	-1.631255	4.094257
K	0.311852	2.865662	4.018307
K	1.793191	-3.248420	0.356710
K	2.237378	-3.520111	-4.104637
K	2.421270	4.024792	0.209536
K	3.403361	0.265104	-2.012102
K	3.662598	0.281356	2.427934

Na4K1
energy = -2.447552508 eV

Na	-1.705645	-0.931848	-0.827346
Na	0.015198	0.535274	2.043359
Na	0.889964	-2.715430	0.854274
Na	1.782178	0.116689	-1.127961
K	-0.981695	2.995315	-0.942326

Na4K2
energy = -3.108314107 eV

Na	-1.336809	0.669776	-2.027967
Na	2.004442	-0.432338	-1.464087
Na	-2.004436	0.432348	1.464091
Na	1.336802	-0.669786	2.027967
K	-0.925024	-2.999164	-0.380778
K	0.925025	2.999164	0.380774

Na4K3
energy = -3.747346315 eV

Na	-0.350252	0.981346	-1.565167
Na	0.210130	-2.625299	-1.786533
Na	0.416534	-1.046816	1.505380
Na	2.955239	-0.501458	-1.069205
K	-3.269977	-1.561133	-0.214590
K	-2.131672	2.105657	1.923168
K	2.169998	2.647703	1.206947

Na4K4
energy = -4.418719611 eV

Na	-2.296839	-0.136117	0.694919
Na	-0.219708	2.023106	-1.278871
Na	0.956175	-0.800862	2.054528
Na	1.560327	-1.086128	-1.470556
K	-2.052183	-1.016210	-3.209562
K	-0.875422	-3.842275	0.126318
K	-0.466165	2.904614	2.625154
K	3.393815	1.953873	0.458071

Na4K5
energy = -5.088348274 eV

Na	-2.535751	-0.096065	-1.592117
Na	-0.982778	0.784576	1.438305
Na	0.824028	1.063504	-2.250431
Na	1.877051	-1.340707	0.113715
K	-1.604744	-3.113493	1.112806
K	-1.530852	3.917393	-0.861829
K	0.003850	-2.809974	-3.089781
K	1.412414	-0.962987	4.019741
K	2.536782	2.557752	1.109590

Na4K6
energy = -5.788816947 eV

Na	-0.262527	0.045725	-0.087973
Na	1.008858	-0.551093	3.086996
Na	2.409453	2.219085	0.347882
Na	3.147733	-1.314283	0.280422
K	-3.079962	-1.241974	2.206642
K	-2.935292	-1.054258	-2.567231
K	-1.129083	2.939891	2.396028
K	-0.824712	3.218802	-2.203859
K	-0.015752	-3.809192	-0.070216
K	1.681284	-0.452703	-3.388690

Na4K7
energy = -6.537247979 eV

K	-2.610801	0.278479	-2.928673
K	2.224258	1.458403	-2.928022
K	0.688128	-2.849946	-2.677172
K	3.813293	-0.868493	0.683755
K	-3.092333	-2.331148	0.700991

K	1.754020	3.045873	1.765532
K	-0.109151	-0.439694	3.909345
Na	-0.853481	3.411558	-1.217624
Na	0.056116	-0.032859	-0.032802
Na	0.741206	-3.384294	1.306016
Na	-2.611256	1.712121	1.418653

Na4K8
energy = -7.253021500 eV

K	-3.616800	-1.585436	0.901281
K	-3.099361	2.627240	-0.452365
K	-1.702009	1.403794	3.678405
K	-0.338963	-3.959125	-0.960983
K	0.001382	-2.660429	3.364562
K	0.829277	4.014053	1.193169
K	3.495587	-2.347829	0.701843
K	3.958176	1.720875	-0.802598
Na	-1.850143	-0.572392	-2.628766
Na	0.211114	0.060953	0.356360
Na	0.350514	2.332146	-2.545479
Na	1.761227	-1.033851	-2.805429

Na4K9
energy = -8.076577534 eV

K	-3.928827	-1.279926	-0.780880
K	-3.040525	1.573798	2.515229
K	-2.470171	2.852955	-1.783201
K	-0.859417	-0.727228	-4.019133
K	-0.490686	-4.093679	-1.024269
K	0.548771	3.938981	1.366318
K	1.948718	2.545790	-2.672508
K	3.117145	-1.769687	-2.198902
K	3.954608	1.087557	1.107458
Na	-1.533354	-2.190946	2.403545
Na	-0.014667	0.049610	-0.090001
Na	0.733940	0.451721	3.490819
Na	2.034464	-2.438946	1.685527

Na4K10
energy = -8.747981289 eV

K	-1.017231	-2.305194	-5.174088
K	1.097372	3.288640	-2.345672
K	4.198967	0.985823	-0.068692
K	-2.605781	3.433047	0.178811
K	2.667126	-3.216903	0.244078
K	-4.081417	-0.789892	0.489606
K	1.408520	3.697891	2.161664
K	-1.022959	-3.126673	2.790170
K	2.399131	-0.407513	3.795995
K	-1.859650	1.124108	3.950889
Na	1.639330	-0.680204	-2.702328
Na	-1.867033	0.580781	-2.574763
Na	-1.051447	-2.799321	-1.229197
Na	0.095072	0.215410	0.483526

Na4K11
energy = -9.451430188 eV

Na	-0.468008	0.493787	-3.069362
Na	0.248724	-2.673487	-1.224955
Na	-2.814129	-0.766189	-0.451033
Na	0.473577	0.587762	0.425645
K	-2.637176	-2.550519	-4.150711
K	3.362166	-0.512052	-2.595502
K	1.744846	3.692915	-2.195953
K	-2.612980	3.208765	-1.085824
K	-3.090959	-4.813277	-0.370768

K	4.257474	1.988541	1.076194
K	3.255061	-2.376430	1.468957
K	0.472381	4.345599	2.032492
K	-0.955145	-2.655784	2.765155
K	-2.757179	1.367534	2.988040
K	1.521348	0.662835	4.387626

Na5K1
energy = -3.187715389 eV

Na	-1.228321	-0.969300	1.993237
Na	-0.841389	2.311118	0.609965
Na	0.990115	-2.279699	-0.493873
Na	1.377028	1.000713	-1.877142
Na	2.074685	0.438258	1.619652
K	-2.372119	-0.501090	-1.851839

Na5K2
energy = -3.825498732 eV

Na	-0.829900	0.724026	2.919373
Na	-0.603179	1.722581	-0.575002
Na	0.693888	-1.666719	0.634284
Na	2.370055	1.459657	1.548921
Na	2.517133	0.315102	-1.816698
K	-3.344688	-1.122071	0.442595
K	-0.803308	-1.432576	-3.153473

Na5K3
energy = -4.494887300 eV

Na	0.118363	-2.160527	-1.467308
Na	1.924948	0.787851	-0.517510
Na	-2.225732	0.343836	-0.318729
Na	-1.482494	-2.458874	1.752204
Na	-0.002016	0.743706	2.506342
K	-0.375945	1.204418	-3.741134
K	-0.488398	3.917739	-0.028680
K	2.531274	-2.378148	1.814817

Na5K4
energy = -5.175543525 eV

Na	1.110222	2.146031	-1.967693
Na	-0.052729	-1.152495	-0.610041
Na	-1.643015	2.114635	0.358530
Na	1.802132	1.362328	1.481906
Na	-1.027774	-0.344096	2.921507
K	-2.278115	0.585674	-3.408565
K	3.817953	-0.745464	-1.420773
K	-3.912362	-1.317727	0.328663
K	2.183688	-2.648888	2.316466

Na5K5
energy = -5.876276233 eV

Na	1.153362	1.089569	-2.435133
Na	1.893054	-2.109416	-0.812350
Na	-0.941446	0.008272	0.369539
Na	2.603493	1.027055	0.927491
Na	1.319648	-1.816636	2.736035
K	-1.309091	-2.052126	-3.245634
K	-2.920295	1.990568	-2.396075
K	0.073896	4.053816	0.141461
K	-1.559081	-3.844868	0.832216

K -0.313540 1.653765 3.882449

Na5K6
energy = -6.617545494 eV

Na	0.958310	3.331319	-0.257603
Na	-0.100061	-0.083786	-0.201598
Na	-1.887160	2.538753	1.741806
Na	1.374225	1.165589	2.789144
Na	-1.800165	-0.850676	2.849303
K	0.547859	1.396585	-3.789951
K	1.406994	-2.858173	-2.597941
K	-3.479482	1.076275	-1.641122
K	3.822763	0.395603	-0.486882
K	-2.488887	-3.206617	-0.370101
K	1.645603	-2.904873	1.964946

Na5K7
energy = -7.350368351 eV

Na	-1.244452	1.652519	-2.808715
Na	-0.297567	-0.160728	0.301662
Na	0.142616	-1.730968	-2.981207
Na	0.343173	3.432977	-0.031835
Na	2.261748	1.107871	-2.093530
K	-3.709625	-1.403936	-1.709056
K	-3.561935	2.398286	0.462597
K	-0.890653	-4.184121	0.181617
K	-0.649858	2.014458	3.721919
K	1.060191	-2.077367	3.565077
K	3.197957	-2.461076	-0.410326
K	3.348405	1.412087	1.801797

Na5K8
energy = -8.174838738 eV

Na	-3.598264	-0.058924	0.335442
Na	-2.009938	1.491818	-2.572514
Na	-1.788493	3.055398	0.727467
Na	-1.449308	0.432453	3.255123
Na	0.097439	-0.054201	-0.019232
K	-2.189666	-2.565253	-2.533857
K	-1.769089	-3.359904	1.837618
K	1.379460	3.576650	-1.760734
K	1.422699	-0.333590	-3.917737
K	1.800004	2.781996	2.610741
K	1.866106	-3.615181	-0.836703
K	2.109445	-1.631222	3.220766
K	4.129606	0.279959	-0.346382

Na5K9
energy = -8.842706097 eV

K	-0.928798	1.374349	-4.190139
K	0.391904	-2.910798	-3.424034
K	3.247471	0.497390	-2.761696
K	-3.673599	-1.581307	-2.086761
K	0.981864	3.928627	-0.920796
K	-3.324968	2.646688	-0.599834
K	3.037268	-2.879855	0.208937
K	-3.398767	-0.775098	2.325977
K	2.167340	1.485146	5.112316
Na	-0.190343	-0.085129	-0.494033
Na	-1.019454	-3.495755	0.376295
Na	2.805755	1.027599	1.216597
Na	-0.600472	2.141520	2.337035
Na	0.504799	-1.373376	2.900134

Na5K10

energy = -9.577780009 eV

K	-4.120828	-3.707762	-0.014284
K	-3.135488	2.801438	-0.782467
K	-1.717810	-3.605578	3.844186
K	-0.748544	2.902934	3.050252
K	-0.283132	1.975435	-4.169219
K	1.008944	4.617984	-0.750611
K	1.339922	-2.162151	-3.438208
K	3.567985	2.139133	2.014574
K	3.726847	-2.060717	0.394498
K	3.849465	1.467630	-2.436184
Na	-2.485082	-0.375959	1.557606
Na	-2.260602	-0.904021	-2.119913
Na	-0.167398	-2.946553	0.182254
Na	0.500376	0.626744	-0.328229
Na	0.925345	-0.768556	2.995745

Na6K1
energy = -3.902447890 eV

Na	2.508901	-0.112237	-1.719862
Na	-0.326676	1.840489	-0.575403
Na	-2.996342	-0.473137	0.251270
Na	0.352710	-1.809224	0.653840
Na	2.429664	1.014036	1.667898
Na	-0.923927	0.794190	2.868644
K	-1.044330	-1.254118	-3.146388

Na6K2
energy = -4.571888944 eV

Na	-0.722859	0.981664	-3.170434
Na	-0.514245	-2.191358	-1.408993
Na	1.947404	0.398502	-0.894593
Na	-3.290812	0.084257	-0.837479
Na	-0.781175	2.535390	0.115424
Na	-1.030177	-0.642075	1.810499
K	2.319468	-2.770634	1.487303
K	2.072396	1.604254	2.898273

Na6K3
energy = -5.247094708 eV

Na	-0.167648	-0.285757	-2.712868
Na	1.811665	1.917519	-0.714453
Na	-2.711040	-0.289268	-0.189938
Na	-0.090277	-2.729879	-0.094809
Na	-0.731727	1.914019	1.808475
Na	1.889029	-0.526599	1.903617
K	-1.817783	3.290958	-1.827952
K	3.479191	-1.641949	-1.635668
K	-1.661411	-1.649043	3.463596

Na6K4
energy = -5.963832453 eV

Na	-0.166690	-0.320795	-0.993045
Na	3.113407	1.355588	-0.820249
Na	0.373755	2.625659	1.205827
Na	-0.055206	-3.277298	1.208272
Na	2.055068	-0.492552	2.085128
Na	-1.566043	-0.210572	2.447650
K	0.160454	3.104996	-2.912845
K	2.989357	-2.642984	-1.366783
K	-3.540658	-2.306484	-0.543482

K -3.363443 2.164443 -0.310472

Na6K5
energy = -6.696930888 eV

Na	2.312980	2.025260	-1.622329
Na	3.136166	-1.423372	-1.140022
Na	-0.123668	-0.121887	-0.127311
Na	-3.161601	1.663159	0.640651
Na	0.113540	3.217633	1.033853
Na	2.674514	0.613491	1.886972
K	-0.200201	-2.359628	-3.246331
K	-1.505773	2.081358	-3.021591
K	-3.252610	-2.381705	0.238468
K	1.003633	-3.425878	1.632047
K	-0.996980	0.111570	3.725593

Na6K6
energy = -7.447116788 eV

Na	-3.015002	0.891366	-0.958216
Na	-2.309180	0.056995	2.520408
Na	-1.000363	3.146890	1.039954
Na	-0.844477	-1.068996	-3.135616
Na	-0.099261	2.454158	-2.439765
Na	0.457441	-0.135176	0.145372
K	-2.700060	-3.035191	-0.094982
K	0.501577	-2.921759	3.057143
K	1.317660	1.344543	3.876570
K	1.599333	-3.765606	-1.181807
K	2.994887	3.056378	0.167130
K	3.097445	-0.023603	-2.996192

Na6K7
energy = -8.271137256 eV

Na	-1.213434	3.204319	-1.019623
Na	0.032852	-0.076149	-0.093806
Na	1.687424	2.945502	1.206981
Na	-1.619957	2.121451	2.456806
Na	-2.001789	-1.521434	2.541206
Na	1.202795	0.040573	3.395860
K	-1.565959	0.226257	-3.843564
K	1.976133	-2.395918	-2.742235
K	2.334862	2.142688	-2.740316
K	-2.164232	-3.360037	-1.141348
K	-4.186740	0.533888	-0.218355
K	4.144470	-0.241647	0.596944
K	1.373575	-3.619493	1.601450

Na6K8
energy = -8.937851898 eV

Na	-1.689221	1.178224	3.041953
Na	-1.397477	-2.403205	2.203332
Na	-0.438429	0.203683	-0.232596
Na	1.521261	-2.868434	0.074731
Na	1.551030	-0.430521	2.856191
Na	3.146865	0.489458	-0.417648
K	-4.482695	-0.338487	0.491731
K	-2.650764	0.717665	-3.546138
K	-2.568789	3.683429	-0.088472
K	-2.043151	-3.366987	-1.724420
K	1.077448	3.132538	-2.689819
K	1.463240	-1.270473	-3.640510
K	1.508557	3.431877	1.801145
K	5.002126	-2.158768	1.870520

Na6K9

energy = -9.669610086 eV

Na	-3.036110	-1.061081	0.420459
Na	-1.696270	-1.272423	-2.963568
Na	-0.155853	-0.876537	2.807757
Na	0.025151	0.740740	-0.450721
Na	0.032976	-2.969189	-0.280379
Na	2.974828	-0.924992	0.786522
K	-3.610160	2.200869	-1.868605
K	-2.491594	2.360143	2.506118
K	-2.367382	-4.228555	2.720207
K	-0.110110	4.750714	-0.521896
K	0.165977	2.152538	-4.274122
K	2.036788	2.478955	2.786795
K	2.170230	-4.168733	2.922002
K	2.405432	-1.583936	-3.162098
K	3.656098	2.401486	-1.428471

Na7K1
energy = -4.643042397 eV

Na	-3.310533	0.440813	0.482931
Na	-1.427565	2.430179	-1.855641
Na	-1.187998	-1.176818	-1.957635
Na	-0.603006	-1.615132	1.594077
Na	-0.197525	1.966909	1.514172
Na	1.741663	0.862049	-1.317898
Na	1.880123	-2.666936	-0.754905
K	3.104842	-0.241064	2.294898

Na7K2
energy = -5.321081038 eV

Na	-1.862539	1.476697	1.423991
Na	-1.674151	-2.056451	0.803658
Na	-0.148420	2.098116	-1.656368
Na	0.038863	-1.414011	-2.272978
Na	0.100262	-0.626011	3.595772
Na	1.734434	1.679910	1.359063
Na	1.922850	-1.853236	0.738738
K	-3.669116	0.143360	-1.930726
K	3.557817	0.551626	-2.061150

Na7K3
energy = -6.047872246 eV

Na	-2.473318	-1.068474	-2.167086
Na	0.738529	-0.007897	-0.832205
Na	0.544742	3.382072	0.469040
Na	-2.511103	1.420390	0.476886
Na	-1.686121	-2.040907	1.241883
Na	1.902207	-2.313318	1.727776
Na	0.148027	0.663836	2.843936
K	-1.041904	2.595980	-3.189937
K	0.488384	-3.824341	-1.770959
K	3.890556	1.192659	1.200665

Na7K4
energy = -6.775147434 eV

Na	-1.752437	-0.179117	2.814369
Na	-0.099078	-3.235964	1.589647
Na	-0.044853	-0.129084	-0.248718
Na	0.400699	2.715608	1.829084
Na	0.416597	3.038437	-1.874699
Na	2.050210	-0.507329	2.611542

Na	3.192670	1.342907	-0.329755
K	-3.223128	-2.291321	-0.789031
K	-3.217481	2.205757	-0.283172
K	-0.436197	-0.352738	-4.021104
K	2.712997	-2.607155	-1.298164

Na7K5
energy = -7.544736851 eV

Na	-3.187566	-0.960674	0.831676
Na	-2.320172	0.237835	-2.516998
Na	-0.958166	-2.893094	-1.283643
Na	-0.226933	-2.574012	2.257899
Na	0.154767	0.467300	0.207325
Na	1.176537	-0.634786	-3.160366
Na	2.470226	-2.372606	-0.209308
K	-2.928114	3.095900	0.349579
K	-1.357310	0.985844	3.932755
K	0.346768	3.340456	-2.646118
K	2.888397	-0.073696	3.151578
K	3.941565	1.381533	-0.914380

Na7K6
energy = -8.368195866 eV

Na	-2.730437	-1.248746	-1.964918
Na	-2.248920	2.359258	-1.500602
Na	-0.001062	-0.017440	0.136561
Na	0.028273	0.461789	-3.617751
Na	0.580369	-2.821360	-2.139769
Na	1.359495	3.016516	-1.388517
Na	3.108092	-0.185295	-1.783550
K	-3.806087	0.293401	1.667099
K	-1.662508	-3.631615	1.182833
K	-0.707425	3.524942	2.103797
K	-0.032007	-0.522723	4.095124
K	2.760969	-2.825858	1.320270
K	3.351247	1.597131	1.889423

Na7K7
energy = -9.031549416 eV

Na	-2.835932	1.067232	-1.806671
Na	-2.563248	-2.079136	-0.034205
Na	-2.419006	1.150852	1.805268
Na	-0.808523	-1.700692	-3.163761
Na	-0.124322	-1.693679	2.747913
Na	0.399461	0.226077	-0.290162
Na	0.787264	-3.424117	-0.318282
K	-3.965069	-1.972487	3.699919
K	-0.708736	4.207222	-0.196135
K	0.502961	2.081339	-3.956409
K	1.221461	2.082566	3.310816
K	3.240015	-1.311568	-2.832027
K	3.543416	2.661766	-0.593676
K	3.730258	-1.295378	1.627412

Na7K8
energy = -9.762353254 eV

Na	1.319333	0.823444	-2.580994
Na	-0.552469	-2.343665	-2.148343
Na	-2.294718	0.917592	-1.576603
Na	2.885409	-2.002811	-0.988290
Na	0.191680	3.221251	0.007505
Na	3.343342	1.421681	0.338361
Na	0.142001	-0.326133	0.792817
K	-1.452514	-0.183699	-5.350713
K	-0.891350	4.012980	-3.724887

K	-3.546332	-2.218012	0.595631
K	0.359816	-4.434984	1.177726
K	-2.982709	1.997025	2.228478
K	3.306508	-1.629010	3.063680
K	1.259869	2.295793	3.785220
K	-1.087866	-1.551451	4.380412

Na8K1
energy = -5.394717914 eV

Na	0.729003	0.566560	-2.651945
Na	0.505084	-2.970827	-2.002598
Na	-2.277640	-0.814725	-1.232719
Na	2.422537	2.673921	-0.269564
Na	-1.172969	2.437262	-0.234304
Na	2.656447	-0.909880	0.024468
Na	-0.362783	-2.281524	1.426214
Na	0.741902	0.970462	2.424626
K	-3.241581	0.328753	2.515823

Na8K2
energy = -6.116100768 eV

Na	-2.731422	-0.812512	0.351370
Na	-1.400852	2.385121	-0.770137
Na	-1.342508	1.527099	2.761270
Na	-0.883502	-0.599169	-2.756545
Na	-0.316191	-3.400354	-0.504712
Na	0.998176	-0.204461	0.601298
Na	1.837886	1.776332	-2.320326
Na	2.512693	-1.802898	-2.159321
K	-0.579763	-2.420841	3.445925
K	1.905482	3.551684	1.351179

Na8K4
energy = -7.626902964 eV

Na	0.374800	0.071543	-3.262009
Na	-2.775470	1.038534	-1.695910
Na	-1.654584	-2.486687	-1.680474
Na	0.178199	3.166793	-1.366471
Na	2.016046	-2.469710	-1.222319
Na	3.122224	1.011238	-1.075494
Na	-0.073349	-0.032763	0.499406
Na	1.789868	2.699418	1.888153
K	-3.786887	-1.175644	1.582262
K	-2.253535	3.009086	1.925427
K	-0.203563	-3.799332	1.936445
K	3.266251	-1.032476	2.470984

Na8K5
energy = -8.457021522 eV

Na	-3.039288	-0.760476	1.719108
Na	-2.481822	2.583863	0.240444
Na	-0.575457	1.586350	3.169532
Na	-0.299400	2.308984	-2.713246
Na	-0.000449	-0.123223	-0.041675
Na	1.062488	3.431082	0.476953
Na	2.824203	0.674587	2.086072
Na	3.018791	1.125856	-1.581354
K	-3.403090	-0.367524	-2.371095
K	-1.321460	-3.879766	-0.461200
K	0.368469	-2.340989	3.423761
K	0.740271	-1.500270	-3.791630
K	3.106744	-2.738477	-0.155669

Na8K6
energy = -9.122404771 eV

Na	0.344693	2.580377	-2.926044
Na	-2.823259	0.826368	-2.211696
Na	0.234750	-0.038843	-0.443000
Na	-1.472594	3.247511	0.186892
Na	2.180999	2.953618	0.253805
Na	-2.945137	0.148556	1.361877
Na	-0.152356	-2.281657	2.277968
Na	0.161454	1.469151	2.892422
K	-0.030865	-1.293260	-4.296602
K	3.759175	0.317845	-2.429319
K	-2.507431	-3.105913	-0.948148
K	2.004278	-3.620997	-0.943836
K	3.527100	-0.540679	2.024941
K	-2.280809	-0.662078	5.200738

Na8K7
energy = -9.850654030 eV

Na	-0.548910	0.595660	-2.880977
Na	2.024746	-1.887280	-2.392266
Na	-1.501550	-2.743939	-1.897505
Na	2.606188	1.507881	-1.160274
Na	-3.206879	0.095661	-0.344647
Na	-0.677124	2.868956	0.141430
Na	1.044508	-4.037466	0.453941
Na	0.216760	-0.569586	0.558646
K	0.838053	4.371756	-3.263168
K	-3.533778	3.309599	-2.649825
K	4.237562	-1.506910	1.005713
K	-2.678869	-3.187137	1.976146
K	2.246446	2.160247	2.836587
K	-2.153703	1.091312	3.453964
K	1.086549	-2.068754	4.162233

Na9K1
energy = -6.183398359 eV

Na	-3.414466	-1.511922	0.558667
Na	-1.920803	1.135416	2.595883
Na	-0.839400	0.485837	-0.792708
Na	-0.716145	-3.089159	-1.343593
Na	-0.156738	-2.009597	2.095486
Na	0.951811	-0.723416	-3.581529
Na	1.671393	1.115732	1.975182
Na	2.404076	1.916411	-1.505001
Na	2.438477	-1.540938	-0.365333
K	-0.418204	4.221634	0.362945

Na9K2
energy = -6.925363903 eV

Na	-2.734324	1.066446	-1.133229
Na	-2.376686	-1.506706	1.406831
Na	-1.428070	1.982438	2.209319
Na	-1.295067	-2.217006	-2.063552
Na	0.037177	3.467868	-0.833998
Na	0.118575	0.896403	-3.450445
Na	0.621402	0.053530	-0.033263
Na	0.634684	-0.831517	3.410123
Na	0.716167	-3.402977	0.793664
K	2.784048	2.424984	2.064668
K	2.922093	-1.933465	-2.370119

Na9K3
energy = -7.706809531 eV

Na	-2.542636	-2.198640	0.754098
Na	-2.214171	1.132199	2.321846
Na	-1.459302	-2.071039	-2.762811
Na	-0.056668	0.222160	-0.410111
Na	0.303574	-1.478461	2.897739
Na	0.840439	-3.323812	-0.213142
Na	1.383610	1.965840	2.467549
Na	2.739990	2.383084	-0.930193
Na	3.239995	-0.778653	0.834038
K	-3.813747	0.993049	-1.503225
K	-0.862805	4.123065	-0.215402
K	2.441722	-0.968793	-3.240384

Na9K4
energy = -8.546958839 eV

Na	-1.398843	-3.185913	0.825360
Na	-0.114226	0.058865	0.004424
Na	-0.111554	-0.886298	3.462650
Na	0.444955	0.714481	-3.475560
Na	0.757715	-2.743607	-2.163273
Na	1.732248	3.014068	-0.838259
Na	2.197615	-2.592377	1.187740
Na	2.802298	0.908767	2.025462
Na	3.307341	-0.244892	-1.400828
K	-3.735732	0.087776	1.746902
K	-3.024660	-1.325467	-2.498695
K	-2.338730	3.043009	-1.511767
K	-0.518428	3.151589	2.635844

Na9K5
energy = -9.209814081 eV

Na	-2.971319	0.933896	0.962185
Na	-2.238308	-2.614789	0.760069
Na	-2.142149	-0.642625	-2.339211
Na	-0.922399	-0.605866	3.533683
Na	-0.737381	2.834694	-1.376343
Na	-0.082343	2.722123	2.237852
Na	0.427762	-0.197809	0.090256
Na	1.232193	-3.126484	1.994133
Na	2.585333	0.223130	2.921633
K	-4.567518	2.493852	-2.342586
K	0.529186	-3.706970	-2.031861
K	1.546238	0.409286	-3.733971
K	3.172103	2.835395	-0.220312
K	4.168603	-1.557834	-0.455526

Na9K6
energy = -9.939806952 eV

Na	-2.279469	1.856437	0.215936
Na	-2.265179	-1.909712	-0.272188
Na	-1.164012	-0.498031	2.982745
Na	-1.062480	0.274145	-3.047997
Na	0.577548	-3.306862	1.485348
Na	0.653663	-2.864735	-2.165163
Na	0.800932	0.101396	-0.010994
Na	2.490634	-0.592841	3.090210
Na	3.642665	-2.081731	-0.108714
K	-5.044733	-0.300599	2.177346
K	-4.964893	0.284643	-2.323990
K	0.604314	3.116718	2.774935
K	0.693409	3.746580	-1.769545

K	2.993000	0.202570	-3.481474
K	4.324600	1.972021	0.453544

Na10K1
energy = -6.985398097 eV

Na	-3.433507	-0.590470	-0.773898
Na	-1.715743	-1.330844	2.426555
Na	-0.867199	-0.459365	-3.423616
Na	-0.626141	-2.929327	-0.701166
Na	-0.191706	0.718343	-0.148025
Na	0.723839	1.343239	3.226203
Na	1.575922	2.236915	-2.719347
Na	1.860505	-1.772658	1.691365
Na	2.398090	-1.252810	-1.886711
Na	3.217446	1.440704	0.506531
K	-2.941506	2.596273	1.802109

Na10K2
energy = -7.783977397 eV

Na	-0.909671	-1.228074	-3.052628
Na	-0.018310	2.365112	-2.860510
Na	-3.051707	1.121962	-1.184371
Na	1.029601	-3.213786	-0.622648
Na	0.334559	0.282089	-0.015737
Na	-2.392642	-2.194012	0.176044
Na	-0.877863	3.571906	0.497444
Na	3.366153	-1.088921	1.252984
Na	-2.307133	0.733939	2.406797
Na	0.154929	-1.985754	2.794462
K	3.117063	-0.278756	-2.747066
K	1.555021	1.914295	3.355228

Na10K3
energy = -8.633567155 eV

Na	-3.037767	1.782955	-0.579278
Na	-2.265681	-1.414170	-2.372218
Na	-0.414344	1.661775	-3.144547
Na	-0.073493	-3.561865	-0.224168
Na	-0.050229	-0.021209	0.099973
Na	0.217326	3.564929	-0.068122
Na	1.361480	-1.540190	-2.931817
Na	2.450735	1.499925	2.118170
Na	2.873696	1.492214	-1.528575
Na	3.133169	-1.692570	0.281170
K	-3.385353	-1.775680	1.533321
K	-1.507431	1.990105	3.275950
K	0.697892	-1.986219	3.540139

Na10K4
energy = -9.296264810 eV

Na	-3.209226	-0.257258	-0.327077
Na	-1.794998	0.840178	2.915300
Na	-1.037049	-2.532113	1.743438
Na	-0.490047	-2.519192	-1.982447
Na	0.254906	0.387198	-0.023797
Na	1.242509	2.940329	2.248636
Na	1.600046	-0.557314	3.274576
Na	2.320176	-2.641970	0.324540
Na	2.494153	-0.473618	-2.666658
Na	3.782447	0.721767	0.622344
K	-3.818905	-4.164861	-0.600546
K	-2.124635	3.672155	-0.036870

K	-1.273656	1.048590	-3.704360
K	2.054279	3.536110	-1.787080

Na10K5
energy = -10.02627361 eV

Na	-2.977800	-0.627306	-2.617686
Na	-1.719495	2.509669	-1.147272
Na	-0.335709	-0.665335	-0.214488
Na	-0.334016	1.741550	2.360767
Na	-0.053333	-2.899972	-3.026749
Na	0.327508	0.712668	-3.575196
Na	1.365029	-3.762185	0.309355
Na	1.971343	2.109438	-0.665657
Na	2.638614	-0.636208	1.790059
Na	2.956523	-1.185081	-1.803243
K	-3.972865	0.244194	1.346696
K	-2.745761	-3.896810	-0.099668
K	-0.690861	-2.124896	3.558712
K	0.168804	5.407092	0.802577
K	3.402021	3.073183	2.981791

Na11K1
energy = -7.857896486 eV

Na	-3.421991	0.336075	-0.013956
Na	-1.747471	-2.862518	0.684346
Na	-1.686892	-0.192401	3.255529
Na	-1.480347	3.055938	1.506812
Na	-1.402687	-1.263398	-2.626736
Na	-1.161182	2.384184	-2.152131
Na	0.190756	0.185785	0.314335
Na	1.359287	-2.209090	2.598755
Na	1.483230	-2.911194	-1.071518
Na	1.904094	0.354981	-2.812965
Na	3.676470	-0.357900	0.395095
K	2.286734	3.479539	-0.077564

Na11K2
energy = -8.716421805 eV

Na	-3.547876	-0.131445	-0.336212
Na	-1.960980	1.821972	2.367319
Na	-1.828168	-1.873941	2.416979
Na	-1.682830	2.927929	-1.145888
Na	-1.447236	-3.048483	-1.143629
Na	-1.353963	-0.049700	-3.306601
Na	0.066003	-0.035290	0.018710
Na	1.193626	0.159953	3.353905
Na	1.240132	3.159216	1.084935
Na	1.621067	1.984660	-2.475665
Na	1.819919	-1.771084	-2.500023
K	1.798133	-3.445236	1.328852
K	4.082173	0.301448	0.337317

Na11K3
energy = -9.379491811 eV

Na	-2.619002	-2.272267	-1.230609
Na	-1.056065	2.318369	2.654550
Na	-0.708774	0.235022	-3.154910
Na	-0.329144	-3.618509	1.400233
Na	-0.196028	-0.212865	0.330382
Na	0.285901	3.156527	-0.682383
Na	0.616884	-0.839778	3.751904
Na	1.004719	-2.764977	-1.949864
Na	2.518492	1.681255	1.813022
Na	2.754100	0.448793	-1.638265

Na	2.924210	-1.933907	1.108741
K	-3.541486	1.811333	-0.715516
K	-3.342050	-1.145862	2.698346
K	1.688242	3.136864	-4.385631

Na11K4
energy = -10.10903194 eV

Na	-1.159849	-0.022813	-3.467444
Na	2.306246	1.222939	-3.048975
Na	1.634680	-2.396540	-3.031498
Na	-0.529781	2.906211	-1.364171
Na	-1.582291	-3.016737	-1.328438
Na	4.043518	-0.983683	-0.578164
Na	-2.952392	0.199447	-0.303881
Na	0.597220	-0.284360	-0.280032
Na	1.618969	-3.647462	0.430735
Na	-1.231697	-2.067882	2.189645
Na	-0.553815	1.741984	2.328718
K	3.002471	2.864634	0.665394
K	-3.579457	3.983714	0.936391
K	2.483680	-0.811493	3.291873
K	-4.097502	0.312041	3.559848

Na12K1
energy = -8.801078783 eV

Na	-0.055139	-0.917128	-3.432993
Na	0.323864	2.674062	-2.318228
Na	-2.899758	0.885819	-1.867775
Na	-2.191990	-2.646073	-0.935600
Na	1.487058	-3.130512	-0.786214
Na	0.036841	0.002202	-0.019622
Na	-1.588261	3.074630	0.840222
Na	2.100277	2.680137	1.017508
Na	-3.132012	-0.187338	1.668287
Na	2.819197	-0.907269	1.964328
Na	-0.443035	-2.640099	2.348498
Na	-0.069926	0.895490	3.446020
K	3.612884	0.216080	-1.924431

Na12K2
energy = -9.464138255 eV

Na	1.572272	0.357245	-3.303197
Na	-2.062479	1.253920	-3.046101
Na	-0.972003	-2.302118	-2.985672
Na	2.191428	-2.554767	-1.032574
Na	-3.656012	-1.145861	-0.692381
Na	-0.264956	-0.046168	-0.286802
Na	3.131367	0.833479	0.026343
Na	-2.855214	2.264609	0.479737
Na	-1.060667	-3.476876	0.511649
Na	1.408263	-1.589048	2.449398
Na	0.260467	2.070276	2.479328
Na	-2.166694	-0.677271	2.691116
K	0.622188	3.811233	-1.193416
K	3.852040	1.201348	3.902573

Na12K3
energy = -10.19159701 eV

Na	-3.610841	0.576175	-0.119752
Na	-2.635747	-3.017647	0.136009
Na	-2.614044	-0.875200	3.147296
Na	-1.496607	-0.953102	-2.726066
Na	-1.427980	2.507708	2.216910
Na	-0.774092	2.520114	-1.371968
Na	-0.213546	-0.436479	0.514481

Na	0.182718	-3.279373	2.592413
Na	0.865432	0.111021	3.908281
Na	2.081750	2.214648	1.163631
Na	2.216724	0.080611	-1.966414
Na	3.136894	-1.323736	1.325075
K	0.315183	1.605062	-5.151302
K	1.143740	-3.779574	-1.393642
K	2.830415	4.049772	-2.274951

Na13K1
energy = -9.547385798 eV

Na	-0.744698	0.598979	-3.089418
Na	2.763952	-0.249228	-2.397682
Na	0.076307	-2.848961	-2.035937
Na	1.328188	3.009818	-1.201793
Na	-2.915724	-1.302413	-0.510090
Na	-2.114659	2.446554	0.023686
Na	0.329359	-0.099414	0.203943
Na	2.840936	-2.601885	0.473147
Na	3.613706	1.014615	0.988045
Na	-0.630184	-3.221893	1.634847
Na	0.622224	2.639264	2.469330
Na	-2.064545	0.038357	2.829092
Na	1.519443	-0.819603	3.476235
K	-4.624304	1.395809	-2.863405

Na13K2
energy = -10.28785981 eV

Na	-3.409545	-1.776077	-0.149760
Na	-3.312941	1.364409	1.401461
Na	-2.900753	1.190323	-2.229435
Na	-1.306434	-1.793230	-3.143121
Na	-1.139260	3.646281	-0.456412
Na	-0.551589	-3.803218	-0.181076
Na	-0.358500	2.477837	2.921267
Na	-0.000003	-0.000006	0.000005
Na	2.049356	-2.320854	-2.283747
Na	2.216542	3.118693	0.402925
Na	2.402892	-2.689903	1.338738
Na	2.499403	0.450624	2.889880
Na	3.810834	0.135121	-0.510723
K	-1.123895	-1.636824	3.383893
K	1.123894	1.636823	-3.383894

Na14K1
energy = -10.36654959 eV

Na	-3.652128	0.924729	-0.682550
Na	-2.945791	-1.689418	1.796906
Na	-2.512722	-2.454360	-1.556516
Na	-2.308534	1.873684	2.412160
Na	-1.550303	0.534262	-3.459753
Na	-0.210889	-0.828584	3.745579
Na	-0.011143	0.079924	-0.019673
Na	0.449239	-3.222547	0.793111
Na	0.655172	-2.358438	-2.961257
Na	1.136795	2.432116	2.729735
Na	1.895044	1.092679	-3.142271
Na	2.957055	-0.732660	2.340914
Na	3.238550	2.041608	-0.047513
Na	3.390032	-1.497610	-1.012508
K	-0.530375	3.804616	-0.936364

Part II

Structures obtained at the MP2 level (frozen core)

K6-mp2-Def2-SVP

energy = -3594.5232852378 hartree

K	19.0	-2.1864638363	-0.0398993954	-0.6096499645
K	19.0	-1.0402503788	-0.4771037752	3.7618815405
K	19.0	-0.1942345530	3.9024068659	0.4412201821
K	19.0	0.1942314077	-3.9024042538	-0.4412218830
K	19.0	1.0402537174	0.4771011868	-3.7618819177
K	19.0	2.1864636429	0.0399003718	0.6096500426

K8-mp2-Def2-SVP

energy = -4792.7298314717 hartree

K	19.0	-4.0038466434	-0.5792449267	1.0085288968
K	19.0	-1.7427428784	2.6073531580	-1.3055428455
K	19.0	-1.1167680935	-2.2792415153	-2.2577432220
K	19.0	-0.4801159882	-3.5000869667	2.2140318279
K	19.0	-0.2206471310	1.0623117918	3.2191002284
K	19.0	1.9146284124	0.8189904545	-3.6123062360
K	19.0	2.5694135131	3.2603769739	0.3895416832
K	19.0	3.0800788089	-1.3904589696	0.3443886673

Na1K7-mp2-Def2-SVP-a

energy = -4355.5126193831 hartree

Na	11.0	1.1510953497	0.1290147644	-2.0751688045
K	19.0	-1.9041557996	-2.3314465035	-2.8035838933
K	19.0	-2.6936265616	1.9576282027	-0.9841464624
K	19.0	1.4056589113	3.9112413689	-0.4938148666
K	19.0	4.1093984657	0.1802119194	0.7737396076
K	19.0	1.0554653279	-3.2164912447	0.7728837239
K	19.0	-3.2291825429	-1.7338593328	1.7849178639
K	19.0	0.1053468495	1.1037008255	3.0251718313

Na1K7-mp2-Def2-SVP-b

energy = -4355.5109568341 hartree

Na	11.0	-2.4723299686	-1.3182421566	1.3939844917
K	19.0	-2.3163840262	-2.5378629341	-2.5310055025
K	19.0	-2.7935179165	1.9847887012	-0.9867419266
K	19.0	1.2768351459	3.8552349514	-0.2213919192
K	19.0	3.9318326292	0.1912145036	1.0229613437
K	19.0	1.0442517590	-3.3116176792	0.8119596511
K	19.0	1.3719547665	0.0228126702	-2.8598677361
K	19.0	-0.0426423892	1.1136719436	3.3701005980

Na1K9-mp2-Def2-SVP

energy = -5553.7021252089 hartree

Na	11.0	0.0000118376	0.0000677937	-0.0000530812
K	19.0	-3.4073291857	0.8111342138	-2.0501203911
K	19.0	-2.6391051162	2.2530534956	2.3441090472
K	19.0	-2.0936933645	-2.4001091159	2.5154951210
K	19.0	-1.3709629615	-3.4114636345	-2.0049955325
K	19.0	0.2834167084	3.9456470425	-0.9075232231
K	19.0	1.1534627931	0.0601058097	-3.8907760488
K	19.0	1.5970320931	0.7342010650	3.6580734339
K	19.0	2.4669891277	-3.1510212940	0.6749062203
K	19.0	4.0101780681	1.1583846237	-0.3391165457

Na4-mp2-Def2-TZVPP

energy = -647.4541776850 hartree

Na	11.0	-0.2383712928	-0.0073498891	-0.1689472454
Na	11.0	-0.8053783484	0.0073500641	3.4195619554
Na	11.0	2.9568445682	0.0073501546	-1.8908030804
Na	11.0	2.3898380731	-0.0073503296	1.6977073702

Na5K1-mp2-Def2-TZVPP

energy = -1408.4311050680 hartree

Na	11.0	0.0852404664	-0.1060531232	-0.0230794273
Na	11.0	0.0344929476	-0.0890249550	3.6196960801
Na	11.0	3.5615478926	-0.2001169938	-1.1046415038
Na	11.0	3.4842035521	-0.1792604225	4.7849505719
Na	11.0	5.6639978066	-0.2447755025	1.8707206466
K	19.0	2.6384353347	2.5116229972	1.8207006325

Na6-mp2-VTZ

energy = -971.2090822579 hartree

Na	11.0	0.0287958967	0.0871227206	-0.0673464999
Na	11.0	-0.0255947920	0.1116085876	3.6621333513
Na	11.0	3.5922070026	-0.0097580032	-1.1775878712
Na	11.0	3.5084697960	0.0089943106	4.8602552100
Na	11.0	5.7491019308	-0.0460839165	1.8652850162
Na	11.0	2.6149381659	1.5405083010	1.8256077936

Na7K1_mp2-Def2-SVP-a

energy = -1732.1983194431 hartree

Na	11.0	-3.2480671036	0.3415019031	0.5356621022
Na	11.0	-1.3061758118	2.3936280137	-1.8760979138
Na	11.0	-1.2910121537	-1.2363188785	-2.0914518870
Na	11.0	-0.6710994065	-1.7317517433	1.7176037887
Na	11.0	-0.1857987406	2.0098953817	1.5602415464
Na	11.0	1.8618278744	0.9443699242	-1.4284048527
Na	11.0	1.7094592931	-2.5865489658	-0.8235819277
K	19.0	3.1308670486	-0.1347756351	2.4060281440

Na7K1_mp2-Def2-SVP-b

energy = -1732.1962634695 hartree

Na	11.0	-3.2275619142	0.2831971040	0.6619870159
Na	11.0	-1.3548633601	2.3492692489	-1.7478035176
Na	11.0	-1.2004776621	-1.2503215634	-1.9410146544
Na	11.0	-0.7629775222	-1.8547985162	1.9103716839
Na	11.0	-0.1760744745	2.0110268270	1.6442836847
Na	11.0	2.4850723010	-0.2180905695	2.0036958956
Na	11.0	1.7284070944	-2.6206269694	-0.6489565700
K	19.0	2.5084765377	1.3003444387	-1.8825645380

Na8-mp2-VTZ

energy = -1294.9768715211 hartree

Na	11.0	-2.3704103080	0.0129742241	1.1471672839
Na	11.0	-1.9756512294	-1.2635460579	-2.2318884377
Na	11.0	-0.5793328767	-3.1127215356	0.6730759183
Na	11.0	-0.5603106141	1.9052037223	-1.7292683768
Na	11.0	-0.1933096763	2.6830480942	1.8011020401
Na	11.0	1.3259146669	-0.5939558373	2.1964512833
Na	11.0	1.6047591614	-1.3242713123	-1.6144178040
Na	11.0	2.7483428761	1.6932687025	-0.2422229072

Part III

Structures obtained at the MP2 level
(sub-valence correlated, see text)

K5-mp2

energy = -2996.6148853600 hartree

K	19.0	-1.1491987524	-0.5403061331	-0.9777627362
K	19.0	0.7743490203	2.8298078639	1.4296866149
K	19.0	0.7617436102	-4.4233399078	-0.8534066934
K	19.0	2.6492677477	-1.2862895683	1.4455981825
K	19.0	-2.8244893759	3.4500529652	-0.8852197579

Na1K4-mp2-a

energy = -2559.3231957065 hartree

K	19.0	-1.1796603617	-0.5601945057	-0.9575961589
K	19.0	0.7417142928	2.8173337196	1.4541615208
K	19.0	0.7671587526	-4.4309629783	-0.8504124631
K	19.0	2.6697679454	-1.2696439517	1.4198332613
Na	11.0	-2.4941691613	3.0515527877	-0.6390970260

Na1K4-mp2-b

energy = -2559.3206055940 hartree

Na	11.0	-0.7700724115	-0.3666586300	-0.6538291955
K	19.0	0.7751105220	2.8073199508	1.4227592796
K	19.0	0.3591472377	-4.0223108234	-1.0104743198
K	19.0	2.6330118184	-1.2707723227	1.4386417059
K	19.0	-2.7855249167	2.8823470451	-1.0382018602

Na1K4-mp2-c

energy = -2559.3209820723 hartree

K	19.0	-1.1482407267	-0.5390312400	-0.9772635651
Na	11.0	0.5678202596	2.4758978138	1.1743682521
K	19.0	0.8473291260	-4.3824264690	-0.7807830650
K	19.0	2.5244463561	-1.0723027363	1.4260133553
K	19.0	-2.5796827652	3.5477878513	-0.6834393673

Na2K3-mp2-a

energy = -2122.0286977522 hartree

K	19.0	-1.1764016359	-0.5343481649	-0.9479181591
Na	11.0	0.5680426897	2.4466931797	1.2167581038
K	19.0	0.8262315846	-4.3771472628	-0.7937311855
K	19.0	2.5758913409	-1.0852130558	1.4180268858
Na	11.0	-2.2889525792	3.1581003340	-0.4662465850

Na2K3-mp2-b

energy = -2122.0291804144 hartree

K	19.0	-1.1697811260	-0.5507152389	-0.9504695802
K	19.0	0.8349086251	2.5799571966	1.4396520343
K	19.0	0.9937134408	-4.3119981501	-0.6604576066
Na	11.0	2.2590304865	-1.1989181590	1.1697697357
Na	11.0	-2.4130600264	3.0897593813	-0.5716055233

Na2K3-mp2-c

energy = -2122.0317710639 hartree

K	19.0	-1.1930333532	-0.6622223606	-0.9956632361
K	19.0	0.7680726679	2.6988135334	1.4331138153
Na	11.0	0.7357663431	-3.9897739102	-0.7339303315
K	19.0	2.6664759325	-1.3943039352	1.3797637909
Na	11.0	-2.4724701902	2.9555717028	-0.6563949785

Na2K3-mp2-d

energy = -2122.0286898395 hartree

Na	11.0	-0.8082621824	-0.4263911278	-0.6441398251
K	19.0	0.7157017459	2.7934069623	1.4292305075
K	19.0	0.4054122760	-4.0658814659	-0.9838070552
K	19.0	2.6471525793	-1.2282402180	1.4150480522
Na	11.0	-2.4551930188	2.5351908793	-0.7894426194

Na2K3-mp2-e

energy = -2122.0270488244 hartree

Na	11.0	-0.5831023237	-0.3074432608	-0.4733124153
Na	11.0	0.9615103187	2.3172343978	1.4268797424
K	19.0	0.2608694646	-3.9808287353	-1.0518832350
K	19.0	2.7243528721	-1.3690060081	1.4024021377
K	19.0	-2.1895339518	3.1890413163	-0.5237014498

Na3K2-mp2-a

energy = -1684.7344210094 hartree

Na	11.0	-0.7768083526	-0.4039703453	-0.6787932850
K	19.0	0.8101263347	2.6050280135	1.4092569003
Na	11.0	0.6252074779	-3.5208099173	-0.7084637239
Na	11.0	2.1801174245	-1.1899982539	1.2271884596
K	19.0	-2.7920100044	2.8438122630	-1.0279186809

Na3K2-mp2-b

energy = -1684.7350612106 hartree

Na	11.0	-2.1567321845	1.3063176595	-2.7580067362
Na	11.0	1.7756442404	-1.5411392004	1.2029622457
Na	11.0	-0.6874656195	0.8890279940	0.2613160343
K	19.0	0.6040446692	0.9129275394	3.9105097943
K	19.0	0.4645078944	-1.5671339927	-2.6167823382

Na3K2-mp2-c

energy = -1683.9157422423 hartree

Na	11.0	-0.7596947906	-0.4750319601	-0.6496629969
Na	11.0	0.6145661167	2.3022296037	1.1350947474
K	19.0	0.6234979808	-4.2695181336	-0.8617561638
Na	11.0	2.2208655169	-1.2037192118	1.1855935652
K	19.0	-2.7313783538	3.0407156918	-0.9623498619

Na3K2-mp2-d

energy = -1684.7346864980 hartree

K	19.0	-0.7384089452	-0.5608314249	-0.8699045400
Na	11.0	1.6622973669	1.8335603161	1.2702694420
Na	11.0	0.9169694096	-4.0860361831	-0.6223369109
Na	11.0	2.5608815348	-1.6405908763	1.0255256708
K	19.0	-1.3253114362	3.7034196982	-0.2230976419

Na3K2-mp2-e

energy = -1684.7372235905 hartree

K	19.0	-1.1503240672	-0.4537994126	-0.9057783813
K	19.0	1.0245053427	2.7111967437	1.3834853973
Na	11.0	0.8976029267	-3.7320136116	-0.5231639448
Na	11.0	2.3036404197	-1.1360556882	1.1599251844
Na	11.0	-2.2450437718	3.2305084189	-0.6067473657

Na4K1-mp2-a

energy = -1247.4408560505 hartree

Na	11.0	-0.7747506824	-0.4759516248	-0.7135543144
Na	11.0	0.5902236460	2.1997911831	1.1189995655
Na	11.0	0.6625844545	-3.5708897821	-0.6401951877

Na	11.0	2.1271108281	-1.0663040011	1.1359943178
K	19.0	-2.6051682464	2.9133542251	-0.9012443814

Na4K1-mp2-b

energy = -1247.4427531267 hartree

K	19.0	-1.2203566462	-0.5699352982	-1.0161989625
Na	11.0	0.6141639199	2.2457276051	1.1326189715
Na	11.0	0.9620095371	-3.7537056829	-0.5105002733
Na	11.0	2.1075492451	-1.0226495987	1.1354445744
Na	11.0	-2.1802209859	3.1728924946	-0.5447290100

Na4K1-mp2-c

energy = -1247.4428826016 hartree

Na	11.0	-0.7968041215	-0.3150503697	-0.6496506418
K	19.0	0.8651351008	2.6035582454	1.5402099958
Na	11.0	0.5484611103	-3.4659396929	-0.7213133400
Na	11.0	2.1912622713	-1.1669611809	1.1914708677
Na	11.0	-2.2971094010	2.7248168483	-0.7213094818

Na5-mp2

energy = -810.1486504773 hartree

Na	11.0	-0.8364706452	-0.3971479763	-0.7292628582
Na	11.0	0.5967651415	2.2283185361	1.1329866210
Na	11.0	0.5931501305	-3.5030617873	-0.6682867041
Na	11.0	2.0937959065	-1.0209856467	1.1262655625
Na	11.0	-2.2355682833	2.7228020941	-0.7028070112