Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Material

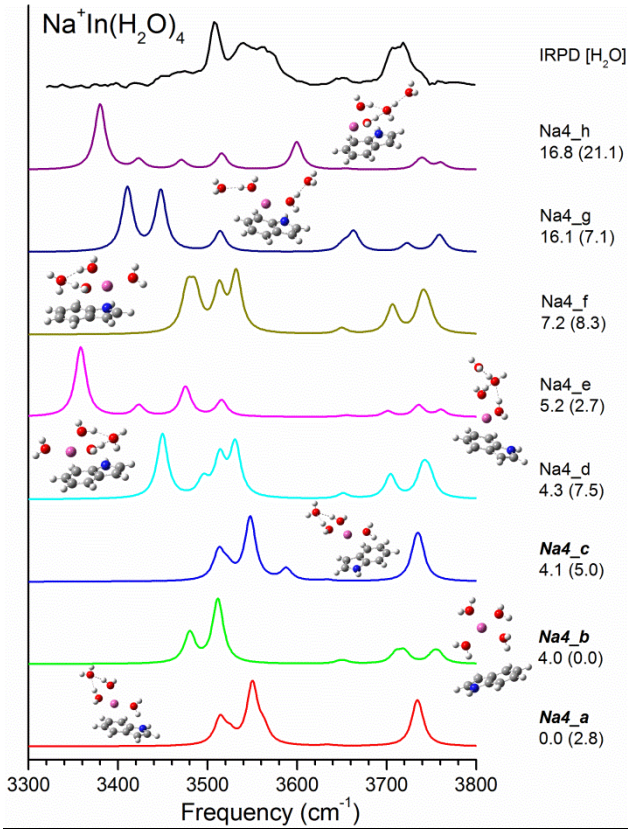

Figure S-1. IRPD spectra in the [H_2O] dissociation channel of Na^+(Indole)(H_2O)$_4$, together with geometries, spectra and relative Gibbs free energies (kJ/mol) of all calculated theoretical structures at 0K and 300K (in parenthesis). The conformers denoted by bold and italic font (Na4_a, Na4_b and Na4_c) are shown in Figure 8 in the paper.

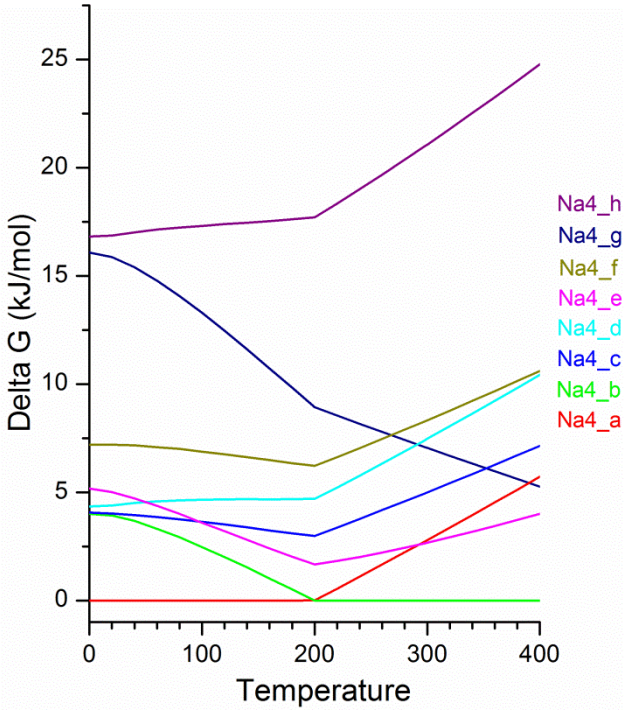

Figure S-2. Relative Gibbs free energies of $Na^+(Indole)(H_2O)_4$ structural conformers as function of temperature.

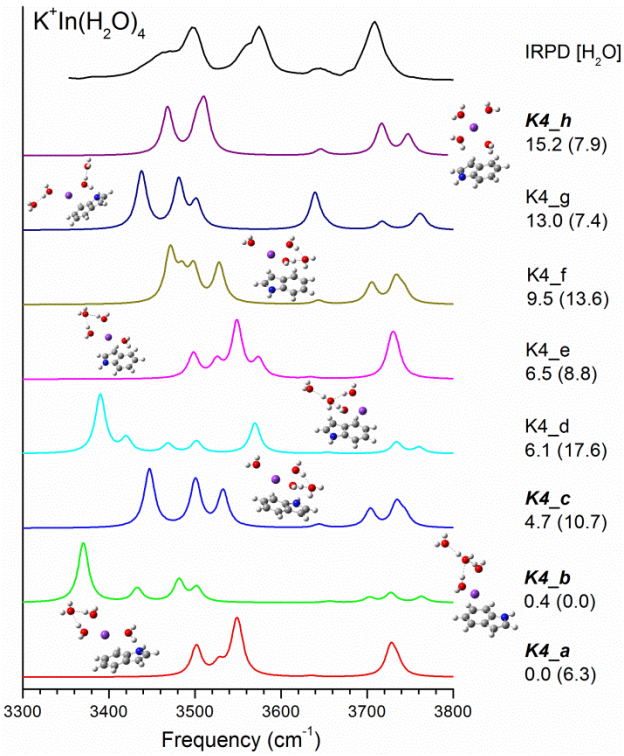

Figure S-3. IRPD spectra in the $[H_2O]$ dissociation channel of $K^+(Indole)(H_2O)_4$, together with geometries, spectra and relative Gibbs free energies (kJ/mol) of all calculated theoretical structures at 0K and 300K (in parenthesis). The conformers denoted by bold and italic font (K4_a, K4_b, K4_c and K4_h) are shown in Figure 9 in the paper.

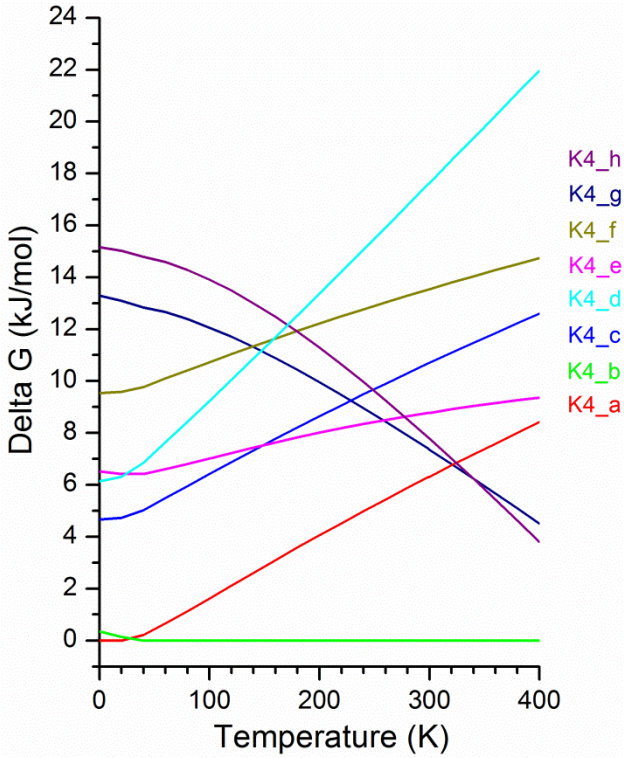

Figure S-4. Relative Gibbs free energies of $K^+(Indole)(H_2O)_4$ structural conformers as function of temperature.

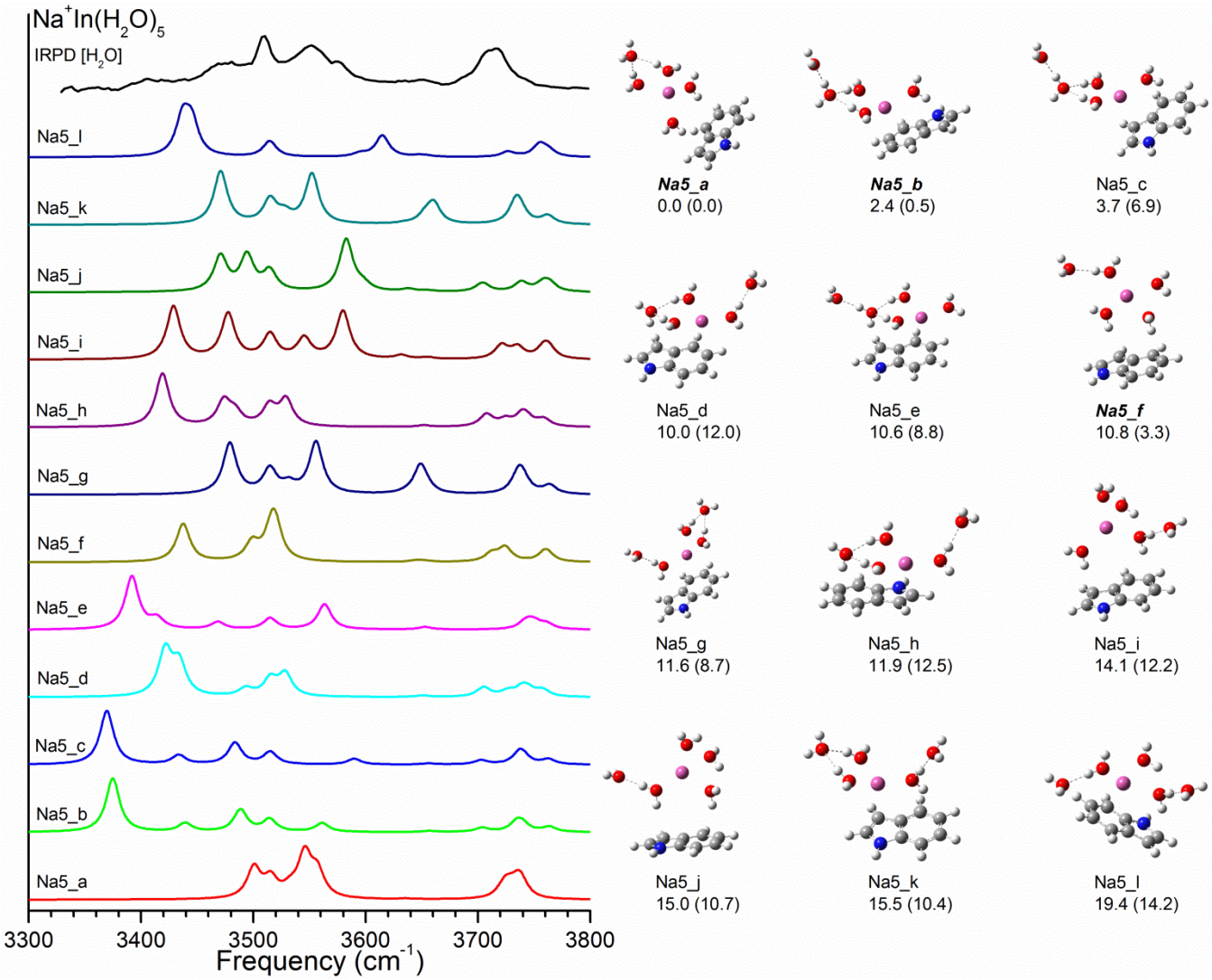

Figure S-5. IRPD spectra in the [H_2O] dissociation channel of Na^+(Indole)(H_2O)$_5$, together with geometries, spectra and relative Gibbs free energies (kJ/mol) of all calculated theoretical structures at 0K and 300K (in parenthesis). The conformers denoted by bold and italic font (Na5_a, Na5_b and Na5_f) are shown in Figure 12 in the paper.

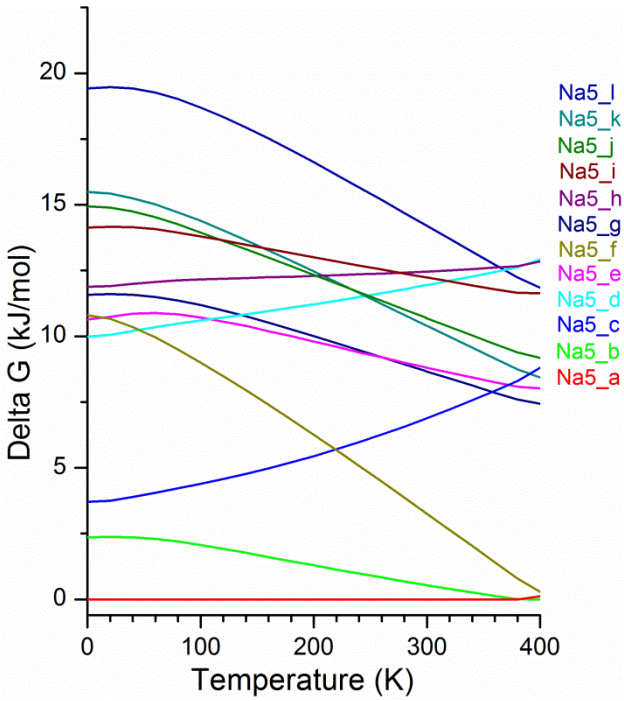

Figure S-6. Relative Gibbs free energies of $Na^+(Indole)(H_2O)_5$ structural conformers as function of temperature.

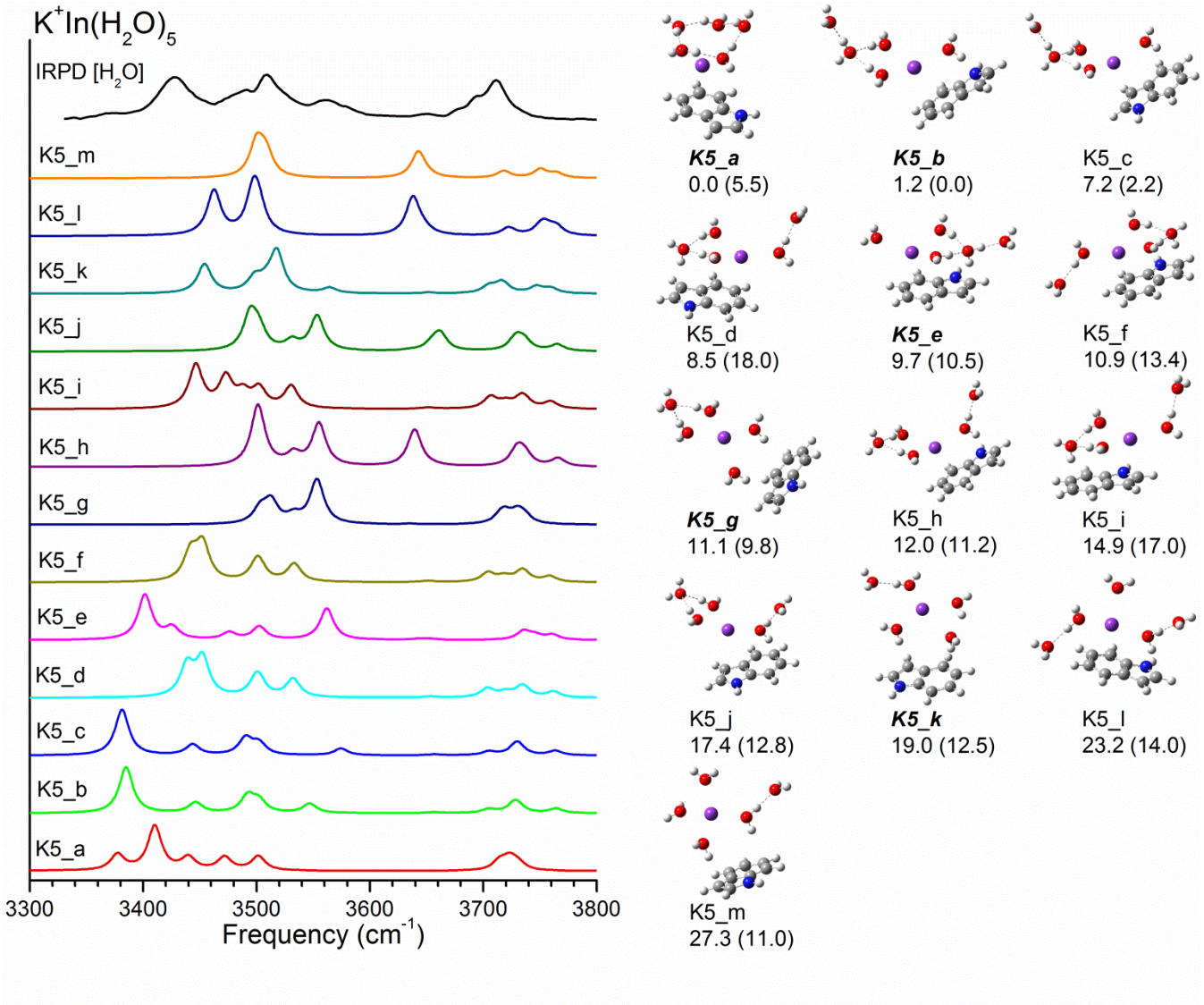

Figure S-7. IRPD spectra in the [H_2O] dissociation channel of K^+(Indole)(H_2O)$_5$, together with geometries, spectra and relative Gibbs free energies (kJ/mol) of all calculated theoretical structures at 0K and 300K (in parenthesis). The conformers denoted by bold and italic font (K5_a, K5_b, K5_e, K5_g and K5_k) are shown in Figure 13 in the paper.

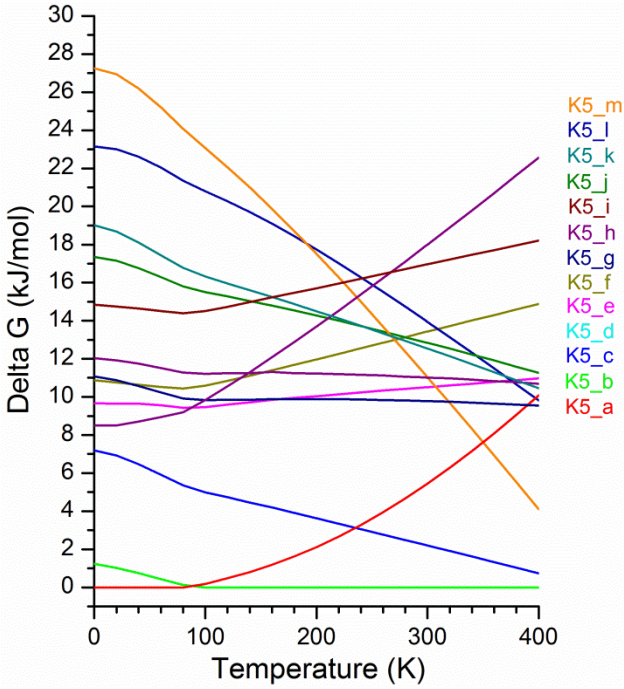

Figure S-8. Relative Gibbs free energies of $K^+(Indole)(H_2O)_5$ structural conformers as function of temperature.

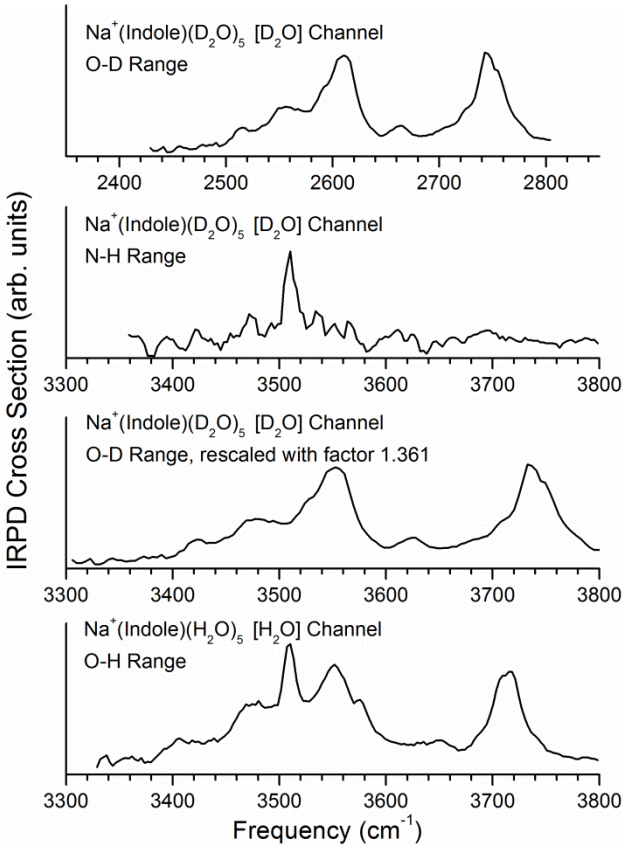

Figure S-9. From top to bottom, (a) IRPD spectra of $Na^+(Indole)(D_2O)_5$ in the $[D_2O]$ dissociation channel and in the OD stretching range (2350 cm^{-1} ~ 2850 cm^{-1}); (b) IRPD spectra of $Na^+(Indole)(D_2O)_5$ in the $[D_2O]$ dissociation channel and in the NH stretching range (3300 cm^{-1} ~ 3650 cm^{-1}); (c) IRPD spectra of $Na^+(Indole)(D_2O)_5$ in the $[D_2O]$ dissociation channel and in the OD stretching range, rescaled to the OH stretching range using the scaling factor of 1.358; (d) IRPD spectra of $Na^+(Indole)(H_2O)_5$ in the $[H_2O]$ dissociation channel and in the OH stretching range (3300 cm^{-1} ~ 3800 cm^{-1}).

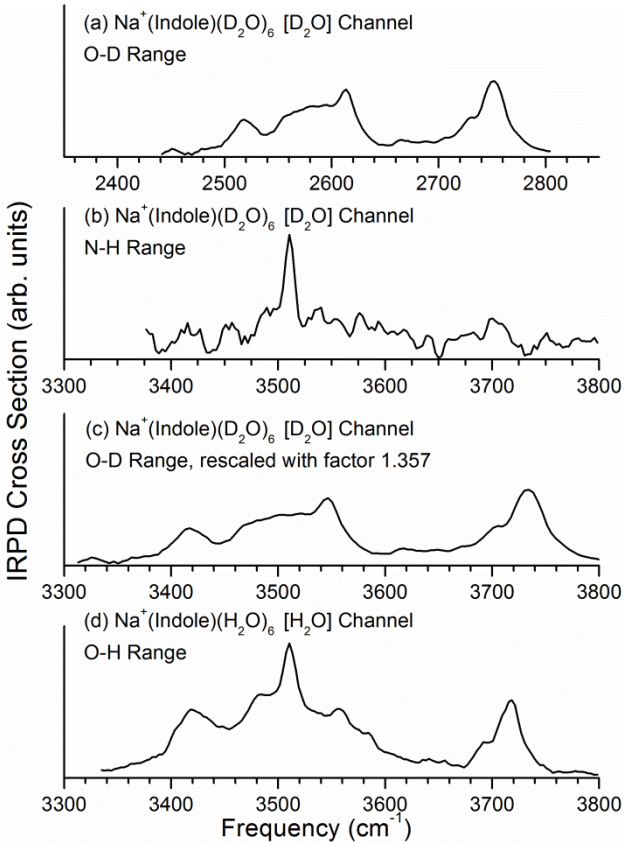

Figure S-10. From top to bottom, (a) IRPD spectra of $K^+(Indole)(D_2O)_6$ in the $[D_2O]$ dissociation channel and in the OD stretching range (2350 cm^{-1} ~ 2850 cm^{-1}); (b) IRPD spectra of $K^+(Indole)(D_2O)_6$ in the $[D_2O]$ dissociation channel and in the NH stretching range (3300 cm^{-1} ~ 3650 cm^{-1}); (c) IRPD spectra of $K^+(Indole)(D_2O)_6$ in the $[D_2O]$ dissociation channel and in the OD stretching range, rescaled to the OH stretching range using the scaling factor of 1.358; (d) IRPD spectra of $K^+(Indole)(H_2O)_6$ in the $[H_2O]$ dissociation channel and in the OH stretching range (3300 cm^{-1} ~ 3800 cm^{-1}).

Table S-1. Coordinates of stable conformations from theoretical calculations.

Na3_a						**K3_a**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.74857	-1.9175	0.379657		1	1	2.759931	-2.14908	0.689591
2	6	2.133374	-1.34546	1.069737		2	6	2.115652	-1.56875	1.345672
3	6	0.554847	0.123518	2.945818		3	6	0.464251	-0.08143	3.141297
4	6	0.752825	-1.61646	1.187205		4	6	0.744006	-1.88051	1.456461
5	6	2.704687	-0.3589	1.874281		5	6	2.640807	-0.53154	2.114866
6	6	1.921563	0.371346	2.801726		6	6	1.822041	0.207558	3.001875
7	6	-0.01563	-0.87348	2.139722		7	6	-0.05994	-1.12919	2.369795
8	1	-0.03629	0.667046	3.678533		8	1	-0.15408	0.467877	3.846962
9	1	3.771347	-0.1628	1.810092		9	1	3.701927	-0.30394	2.058201
10	1	2.397598	1.117968	3.430899		10	1	2.264429	0.993652	3.607499
11	1	0.099669	-3.28402	-0.19182		11	1	0.164406	-3.62284	0.136479
12	7	-1.30719	-1.35008	2.075833		12	7	-1.3366	-1.64935	2.307464
13	1	-2.06794	-1.06774	2.678025		13	1	-2.10924	-1.37976	2.900126
14	6	-1.37577	-2.36571	1.139501		14	6	-1.35941	-2.70261	1.410747
15	6	-0.14365	-2.55184	0.565885		15	6	-0.11352	-2.86843	0.859975
16	1	-2.30991	-2.88031	0.960411		16	1	-2.27291	-3.25641	1.242261
17	8	1.576861	1.254223	-1.99377		17	19	0.80684	1.051248	-0.04589
18	1	2.037632	0.683235	-2.62662		18	8	1.589147	1.567271	-2.54921
19	1	1.305993	2.060524	-2.47823		19	1	2.056824	1.093821	-3.2538
20	8	0.055726	3.117201	0.028939		20	1	1.386871	2.457663	-2.90146
21	1	0.077116	3.552553	-0.848		21	8	-0.06363	3.562432	-0.35437
22	1	-0.36631	3.73748	0.641974		22	1	0.122238	3.981346	-1.21933
23	8	0.487444	3.78912	-2.70878		23	1	-0.51309	4.232652	0.182303
24	1	-0.25967	3.844672	-3.32859		24	8	0.741067	4.272278	-3.02319
25	1	1.077351	4.526307	-2.9413		25	1	0.060926	4.446968	-3.69548
26	11	1.053872	1.102128	0.192587		26	1	1.415156	4.962103	-3.14513
Na3_b						**K3_b**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	-1.20751	-2.245	2.323777		1	1	-1.2877	-1.84355	2.741573
2	6	-0.25544	-2.08463	1.824412		2	6	-0.36205	-1.87313	2.172198
3	6	2.276316	-1.7113	0.550936		3	6	2.100386	-1.99879	0.728063
4	6	0.417934	-0.85181	1.947388		4	6	0.48177	-0.74506	2.124375
5	6	0.33031	-3.10304	1.073047		5	6	0.02518	-3.03553	1.50888
6	6	1.583654	-2.91633	0.440216		6	6	1.242838	-3.09634	0.789842
7	6	1.686867	-0.69277	1.312876		7	6	1.711808	-0.83456	1.406411
8	1	3.249132	-1.58015	0.084213		8	1	3.047929	-2.05822	0.198781
9	1	-0.16413	-4.06785	0.997014		9	1	-0.59932	-3.92302	1.569373
10	1	2.026491	-3.73756	-0.11637		10	1	1.53023	-4.02475	0.303865
11	1	-0.72889	0.611245	3.240539		11	1	-0.34246	0.975567	3.343219

12	7	2.128396	0.58276	1.600307		12	7	2.353788	0.380223	1.545925
13	1	3.02203	0.969956	1.329789		13	1	3.270392	0.605217	1.184909
14	6	1.19745	1.225202	2.390615		14	6	1.585825	1.219786	2.32637
15	6	0.127145	0.389642	2.616758		15	6	0.424367	0.57758	2.691459
16	1	1.383008	2.228335	2.750521		16	1	1.94079	2.210046	2.578565
17	8	-2.89888	-1.50756	-1.17496		17	8	-3.09824	-2.59407	-1.60825
18	1	-3.3481	-0.69913	-0.87934		18	1	-3.67291	-2.51695	-2.38662
19	1	-3.5952	-2.16658	-1.32176		19	1	-3.55537	-3.21536	-1.01904
20	8	0.063222	-1.93816	-3.05856		20	8	0.136972	-1.0967	-3.68601
21	1	0.920387	-2.27031	-3.36923		21	1	0.456917	-0.30794	-4.15261
22	1	-0.51039	-1.92219	-3.84138		22	1	0.24355	-1.82463	-4.31915
23	8	-1.05516	0.826666	-0.40573		23	8	-0.88789	1.315286	-0.21659
24	1	-1.06659	1.653472	-0.91287		24	1	-1.26708	2.179661	-0.43794
25	1	-0.76285	1.064367	0.496622		25	1	-0.49417	1.41362	0.672805
26	11	-0.63421	-1.37806	-0.96374		26	19	-0.80054	-1.20915	-1.12533

Na3_c

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	1	2.290122	-2.09226	0.924126
2	6	1.623416	-1.50956	1.555104
3	6	-0.06847	0.01862	3.278451
4	6	0.413535	-2.06066	2.020444
5	6	1.971454	-0.21811	1.950253
6	6	1.130955	0.53821	2.802866
7	6	-0.40907	-1.2823	2.885254
8	1	-0.70311	0.595179	3.945991
9	1	2.925169	0.20005	1.637445
10	1	1.439276	1.533977	3.108664
11	1	0.146113	-4.20609	1.341336
12	7	-1.50022	-2.06166	3.220126
13	1	-2.24279	-1.79003	3.849537
14	6	-1.38921	-3.29564	2.618835
15	6	-0.23918	-3.33675	1.859381
16	1	-2.1302	-4.06283	2.799924
17	8	-1.71974	-2.46211	-0.81597
18	1	-2.29461	-3.18509	-1.11148
19	1	-1.37641	-2.73869	0.06313
20	8	0.392936	0.681921	-0.76383
21	1	0.662036	1.605947	-0.88263
22	1	0.840169	0.380295	0.054918
23	11	-1.08192	-0.58738	-1.84473
24	8	-1.86756	0.013194	-3.89447
25	1	-1.33874	0.220515	-4.68222
26	1	-2.79194	0.11732	-4.17312

K3_c

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	1	-1.85507	0.1147	2.052172
2	6	-1.52229	-0.26222	1.088231
3	6	-0.70757	-1.30535	-1.44442
4	6	-0.31664	-0.98574	0.982847
5	6	-2.29767	-0.06709	-0.05354
6	6	-1.8923	-0.5812	-1.30886
7	6	0.064587	-1.50715	-0.29098
8	1	-0.41561	-1.72497	-2.40383
9	1	-3.2461	0.458006	0.023883
10	1	-2.53173	-0.43939	-2.17596
11	1	0.706611	-1.2134	2.987753
12	7	1.248591	-2.19301	-0.11164
13	1	1.738659	-2.71565	-0.82416
14	6	1.61674	-2.13408	1.218168
15	6	0.694582	-1.39513	1.921189
16	1	2.505881	-2.64509	1.562278
17	19	0.183427	1.936484	-0.70604
18	8	-0.21991	4.187891	-2.16307
19	1	0.359314	4.966246	-2.20072
20	1	-0.96826	4.405296	-2.7421
21	8	2.228334	1.430233	0.839187
22	1	2.179657	0.592644	1.3325
23	1	3.062208	1.869085	1.117118
24	8	4.569849	2.773224	1.577714
25	1	5.460649	2.606945	1.231924
26	1	4.688625	3.270949	2.401745

Na3_d

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	1	2.530113	-1.74709	0.550221
2	6	1.879549	-1.2318	1.252912
3	6	0.235735	0.104762	3.171315
4	6	0.705838	-1.85598	1.730729
5	6	2.207711	0.035457	1.721165
6	6	1.391531	0.699554	2.667745
7	6	-0.09106	-1.17441	2.698698
8	1	-0.37117	0.604924	3.921575
9	1	3.11591	0.519463	1.373871
10	1	1.689178	1.67838	3.033657
11	1	0.440585	-3.93512	0.868034
12	7	-1.14255	-2.00959	3.020579
13	1	-1.85442	-1.81543	3.711417
14	6	-1.03549	-3.1842	2.306685
15	6	0.075121	-3.13124	1.494271
16	1	-1.74945	-3.98289	2.456629
17	8	-2.54656	-2.21642	-1.38289
18	1	-3.28087	-1.82323	-1.88156
19	1	-2.87207	-3.08005	-1.08211
20	8	0.534212	-1.5988	-2.48435
21	1	1.371666	-1.24398	-2.82284
22	1	0.190279	-2.17444	-3.1861
23	8	-0.85235	0.991606	0.093832
24	1	-1.12848	1.836111	-0.29375
25	1	-0.35919	1.211095	0.906572
26	11	-0.65595	-1.15881	-0.58998

K3_d

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	1	2.255119	-2.31024	0.927676
2	6	1.627163	-1.66882	1.541188
3	6	0.038727	0.016696	3.214659
4	6	0.420719	-2.15333	2.082091
5	6	2.024221	-0.36592	1.838847
6	6	1.235064	0.468607	2.666777
7	6	-0.34953	-1.29685	2.92116
8	1	-0.5558	0.653659	3.864051
9	1	2.978602	0.001564	1.4692
10	1	1.581035	1.472425	2.897079
11	1	0.076017	-4.33044	1.559173
12	7	-1.44584	-2.02202	3.347662
13	1	-2.15544	-1.68986	3.985717
14	6	-1.38537	-3.29791	2.829952
15	6	-0.26598	-3.42032	2.035636
16	1	-2.13603	-4.03168	3.091912
17	8	-2.00431	-2.82391	-0.62356
18	1	-2.6463	-3.5411	-0.7425
19	1	-1.58468	-2.99569	0.246696
20	8	0.514414	0.667294	-0.89558
21	1	0.88206	1.553388	-1.03801
22	1	0.912376	0.356649	-0.05695
23	8	-2.19272	-0.18821	-4.67284
24	1	-1.68244	-0.19388	-5.49893
25	1	-3.08725	0.083093	-4.93547
26	19	-1.28685	-0.79148	-2.17995

K3_e

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	1	2.723063	-1.73055	0.827504
2	6	2.012522	-1.2157	1.469766
3	6	0.20451	0.133443	3.223178
4	6	0.854613	-1.87771	1.930654
5	6	2.24973	0.091957	1.877839
6	6	1.353745	0.761543	2.745202
7	6	-0.03014	-1.18503	2.808948
8	1	-0.46836	0.641388	3.909267
9	1	3.147163	0.60547	1.544937
10	1	1.583684	1.77214	3.072148
11	1	0.74433	-4.01314	1.181452
12	7	-1.05962	-2.05384	3.119926
13	1	-1.80432	-1.86723	3.777119

						14	6	-0.84679	-3.26369	2.489905
						15	6	0.305602	-3.19644	1.74055
						16	1	-1.52612	-4.09053	2.647937
						17	8	-3.31493	-2.2754	-1.64508
						18	1	-3.95677	-1.77435	-2.17382
						19	1	-3.73644	-3.13592	-1.49017
						20	8	0.707369	-1.68137	-2.9485
						21	1	1.503451	-1.16415	-3.15119
						22	1	0.598925	-2.28339	-3.70208
						23	8	-0.73697	1.162962	0.076538
						24	1	-0.9828	2.060697	-0.19447
						25	1	-0.20786	1.265556	0.890237
						26	19	-0.88975	-1.36887	-0.77147

Na4_a

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	1	2.362205	-1.88681	0.13767
2	6	1.831976	-1.33023	0.906643
3	6	0.493556	0.116761	2.975143
4	6	0.623843	-1.82351	1.440051
5	6	2.351068	-0.13449	1.401508
6	6	1.684933	0.584154	2.423669
7	6	-0.02066	-1.08905	2.47986
8	1	-0.00468	0.661281	3.77298
9	1	3.296863	0.240347	1.019197
10	1	2.122803	1.503932	2.800811
11	1	0.014985	-3.78275	0.481975
12	7	-1.16132	-1.78598	2.823026
13	1	-1.80999	-1.52764	3.553478
14	6	-1.2587	-2.92164	2.046087
15	6	-0.19262	-2.97995	1.177253
16	1	-2.07696	-3.61459	2.188587
17	8	1.625093	1.500629	-2.20367
18	1	2.140746	1.013914	-2.86375
19	1	1.63828	2.442039	-2.46941
20	8	-0.20991	3.100048	-0.23997
21	1	0.171822	3.723676	-0.89023
22	1	-0.77615	3.61921	0.350118
23	8	1.22316	4.326263	-2.39114
24	1	0.747139	4.711663	-3.14601
25	1	1.960543	4.932556	-2.20746
26	8	-1.30727	-0.57947	-0.77967
27	1	-1.28787	-1.44186	-0.3219
28	1	-2.07306	-0.59786	-1.3736
29	11	0.375659	0.902846	-0.38893

K4_a

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	1	2.387866	-2.34939	0.421451
2	6	1.895869	-1.68357	1.126088
3	6	0.651257	0.049664	3.025699
4	6	0.615889	-1.99513	1.627122
5	6	2.533367	-0.52782	1.571446
6	6	1.915011	0.332578	2.509592
7	6	0.017925	-1.11993	2.581967
8	1	0.190814	0.698842	3.766112
9	1	3.533081	-0.29365	1.215401
10	1	2.446125	1.215094	2.855628
11	1	-0.1597	-3.95431	0.798514
12	7	-1.20393	-1.66511	2.924924
13	1	-1.84261	-1.28977	3.611992
14	6	-1.3917	-2.84482	2.234599
15	6	-0.30832	-3.08001	1.418795
16	1	-2.28177	-3.43805	2.395941
17	19	0.319919	0.929863	-0.42613
18	8	1.818353	1.868452	-2.46396
19	1	2.451347	1.498616	-3.09758
20	1	1.727798	2.816802	-2.68538
21	8	-0.40165	3.532369	-0.50553
22	1	0.0346	4.083658	-1.18585
23	1	-1.02223	4.113559	-0.04086
24	8	1.15891	4.667326	-2.64867
25	1	0.708464	4.999963	-3.44311
26	1	1.842839	5.325093	-2.43822
27	8	-1.49957	-1.01199	-0.81868
28	1	-1.40709	-1.78232	-0.2245
29	1	-2.24538	-1.21253	-1.40451

Na4_b						K4_b				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.28725	-2.118	0.907138		1	1	2.744811	-2.19906	0.707135
2	6	1.634386	-1.52739	1.545263		2	6	2.114802	-1.59548	1.356042
3	6	-0.02236	0.019834	3.284704		3	6	0.497073	-0.04608	3.129353
4	6	0.428814	-2.06926	2.032108		4	6	0.729213	-1.84763	1.440316
5	6	1.996269	-0.23615	1.927447		5	6	2.670351	-0.58592	2.140309
6	6	1.172916	0.530125	2.787903		6	6	1.868415	0.183852	3.016402
7	6	-0.37648	-1.28132	2.904537		7	6	-0.05797	-1.06597	2.34241
8	1	-0.64298	0.603454	3.959392		8	1	-0.11	0.527631	3.825288
9	1	2.945552	0.176658	1.595148		9	1	3.741037	-0.40362	2.103064
10	1	1.492764	1.52512	3.084665		10	1	2.333069	0.947977	3.633378
11	1	0.134389	-4.2126	1.359776		11	1	0.098128	-3.55425	0.097549
12	7	-1.46772	-2.05152	3.258169		12	7	-1.3551	-1.52815	2.252378
13	1	-2.20058	-1.77181	3.895196		13	1	-2.12751	-1.22365	2.828046
14	6	-1.37358	-3.28865	2.659351		14	6	-1.4077	-2.57395	1.348215
15	6	-0.23416	-3.34092	1.885747		15	6	-0.15982	-2.79289	0.821142
16	1	-2.11841	-4.04923	2.852038		16	1	-2.34192	-3.08425	1.157509
17	8	-1.76816	-2.45552	-0.80065		17	19	0.948026	1.094466	-0.054
18	1	-2.37481	-3.16638	-1.059		18	8	1.804104	1.606728	-2.51746
19	1	-1.40629	-2.7217	0.071807		19	1	2.312096	1.177056	-3.2214
20	8	0.753027	-0.51504	-3.37434		20	1	1.553485	2.495703	-2.85425
21	1	1.399947	0.04274	-2.9112		21	8	-0.0215	3.547255	-0.40656
22	1	1.198118	-0.86793	-4.15995		22	1	0.194428	3.934965	-1.28409
23	8	0.339745	0.697941	-0.74233		23	1	-0.5136	4.224764	0.080234
24	1	0.180411	1.636683	-0.55591		24	8	0.808273	4.188927	-3.01683
25	1	0.793245	0.354259	0.055771		25	1	0.11779	4.26861	-3.69443
26	11	-1.04436	-0.67602	-1.98979		26	1	1.428444	4.942897	-3.17154
27	8	-2.74934	0.304266	-3.15673		27	8	2.529523	6.289504	-3.48263
28	1	-2.63483	0.730825	-4.02106		28	1	3.307417	6.277242	-4.06184
29	1	-3.69484	0.378425	-2.95184		29	1	2.443054	7.199675	-3.15882
Na4_c						K4_c				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	-1.06305	0.418348	2.516731		1	1	2.490357	-2.36745	0.593685
2	6	-0.58878	-0.48425	2.138814		2	6	1.943887	-1.74126	1.293771
3	6	0.64997	-2.88962	1.222006		3	6	0.546694	-0.10444	3.173789
4	6	0.787229	-0.49054	1.824352		4	6	0.626406	-2.07043	1.668946
5	6	-1.32247	-1.65435	1.982055		5	6	2.54561	-0.61918	1.85805
6	6	-0.71063	-2.84442	1.522659		6	6	1.85234	0.192809	2.787874
7	6	1.386938	-1.70786	1.385067		7	6	-0.04733	-1.24458	2.615231
8	1	1.122148	-3.81333	0.897389		8	1	0.025359	0.506604	3.905909
9	1	-2.37986	-1.66462	2.230108		9	1	3.576427	-0.38042	1.608644

10	1	-1.30676	-3.74782	1.428507		10	1	2.358735	1.04401	3.235733
11	1	1.754389	1.524778	2.201453		11	1	-0.05524	-4.01319	0.726168
12	7	2.727178	-1.44904	1.17488		12	7	-1.28678	-1.81041	2.842348
13	1	3.417826	-2.13018	0.891392		13	1	-1.98015	-1.46266	3.48984
14	6	2.994144	-0.12786	1.466144		14	6	-1.41196	-2.96158	2.09514
15	6	1.834173	0.500553	1.860238		15	6	-0.27004	-3.15267	1.347199
16	1	4.001823	0.257719	1.390645		16	1	-2.29907	-3.57532	2.179424
17	8	1.680569	2.209254	-2.07605		17	19	0.790939	1.218271	-0.23886
18	1	2.440398	2.070599	-2.66084		18	8	-1.76605	-1.7173	-1.14616
19	1	1.392851	3.13661	-2.19772		19	1	-2.44627	-2.24748	-1.59235
20	8	-0.8731	2.708405	-0.31445		20	1	-1.47726	-2.23694	-0.36358
21	1	-0.661	3.533715	-0.7956		21	8	0.579384	-0.55072	-2.23323
22	1	-1.73342	2.842986	0.110317		22	1	0.994934	-0.86583	-3.04937
23	8	0.325291	4.724795	-1.94869		23	1	-0.22406	-1.09383	-2.09497
24	1	-0.13368	5.081563	-2.72787		24	8	-1.87662	0.950247	-0.20372
25	1	0.754034	5.487094	-1.52409		25	1	-2.11017	0.06938	-0.56386
26	8	-0.24714	-1.09091	-1.48008		26	1	-2.70183	1.451934	-0.13075
27	1	-0.38225	-1.81822	-0.84421		27	8	1.99164	3.608592	-0.78696
28	1	-0.68823	-1.36016	-2.30005		28	1	2.599198	4.137837	-0.24589
29	11	0.474445	0.899339	-0.65125		29	1	1.886979	4.111623	-1.61067
Na4_d						**K4_d**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.33378	-2.23437	0.525443		1	1	2.460412	-2.58789	0.759596
2	6	1.770118	-1.69525	1.28195		2	6	1.937988	-1.88518	1.403233
3	6	0.335867	-0.29374	3.31806		3	6	0.603151	-0.05003	3.140112
4	6	0.497108	-2.14629	1.681795		4	6	0.587849	-2.09944	1.746594
5	6	2.306567	-0.56232	1.893052		5	6	2.600969	-0.77639	1.925179
6	6	1.593375	0.133354	2.900302		6	6	1.938509	0.134488	2.783705
7	6	-0.19372	-1.43761	2.707282		7	6	-0.05449	-1.17621	2.624535
8	1	-0.20067	0.231113	4.103816		8	1	0.105271	0.635693	3.820722
9	1	3.310358	-0.23591	1.629805		9	1	3.653528	-0.62456	1.700111
10	1	2.048561	0.996062	3.379209		10	1	2.490001	0.973076	3.200771
11	1	-0.09458	-4.05414	0.61346		11	1	-0.20582	-4.02886	0.869819
12	7	-1.38571	-2.09929	2.928052		12	7	-1.3365	-1.64049	2.837368
13	1	-2.07418	-1.85061	3.624851		13	1	-2.02271	-1.21099	3.441816
14	6	-1.46499	-3.19705	2.098526		14	6	-1.52012	-2.81978	2.145163
15	6	-0.33965	-3.25801	1.305126		15	6	-0.37268	-3.13148	1.451564
16	1	-2.30993	-3.87011	2.159219		16	1	-2.45301	-3.36176	2.225702
17	8	-1.72745	-1.57778	-1.07363		17	19	0.840245	0.858726	-0.24623
18	1	-2.46895	-1.97725	-1.557		18	8	-1.86137	-1.72625	-1.2207
19	1	-1.509	-2.19104	-0.33752		19	1	-2.57634	-2.21096	-1.69697
20	8	0.748033	-0.5415	-1.93425		20	1	-1.64797	-2.25438	-0.42605
21	1	1.212042	-0.77675	-2.75111		21	8	0.581685	-0.85198	-2.23802
22	1	-0.09712	-1.03757	-1.92468		22	1	0.963349	-1.20546	-3.05462

23	8	-1.31628	0.972329	0.015624		23	1	-0.28362	-1.30022	-2.10316
24	1	-1.76276	0.188931	-0.36861		24	8	-1.80359	0.907473	-0.32023
25	1	-2.00491	1.599878	0.278684		25	1	-2.0784	0.033452	-0.6798
26	11	0.935898	0.839058	-0.13598		26	1	-2.5917	1.469723	-0.30434
27	8	2.154506	2.743006	-0.48873		27	8	-3.85832	-3.15216	-2.51488
28	1	2.853869	3.151027	0.046374		28	1	-4.79308	-2.90035	-2.57602
29	1	2.036722	3.331317	-1.25173		29	1	-3.70574	-3.79804	-3.22243
Na4_e						**K4_e**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	3.072085	-1.4723	0.525369		1	1	-1.69384	-0.98947	2.859522
2	6	2.293263	-1.0675	1.166445		2	6	-0.95715	-1.54886	2.288399
3	6	0.275963	-0.02768	2.904975		3	6	0.975073	-3.07202	0.834691
4	6	0.957302	-1.50079	1.027405		4	6	0.346173	-1.04162	2.10898
5	6	2.606784	-0.13667	2.157423		5	6	-1.27779	-2.79002	1.744262
6	6	1.606833	0.379703	3.017474		6	6	-0.31933	-3.54389	1.02486
7	6	-0.03447	-0.97015	1.912448		7	6	1.293475	-1.82256	1.384416
8	1	-0.48377	0.354211	3.582092		8	1	1.712072	-3.66009	0.294246
9	1	3.637052	0.181912	2.289899		9	1	-2.26927	-3.20607	1.903189
10	1	1.883096	1.087869	3.793526		10	1	-0.59581	-4.51636	0.627706
11	1	0.738965	-3.04557	-0.60766		11	1	0.629047	0.949168	3.152665
12	7	-1.23147	-1.56938	1.583388		12	7	2.480541	-1.1109	1.366632
13	1	-2.10571	-1.44383	2.074347		13	1	3.363633	-1.46086	1.021542
14	6	-1.02806	-2.46114	0.546311		14	6	2.323226	0.063607	2.081853
15	6	0.29118	-2.44163	0.169776		15	6	1.028784	0.153847	2.536748
16	1	-1.8516	-3.0474	0.162025		16	1	3.160452	0.733339	2.226071
17	8	0.464352	1.440989	-1.74713		17	19	0.200794	1.086321	-0.52654
18	1	0.233149	0.801312	-2.43639		18	8	1.718393	1.953719	-2.58463
19	1	0.455865	2.334923	-2.15681		19	1	2.263571	1.559439	-3.28195
20	8	1.156577	3.604115	0.422028		20	1	1.673357	2.911565	-2.77949
21	1	0.997482	4.027758	-0.45193		21	8	-0.31086	3.733452	-0.51369
22	1	1.385605	4.308125	1.046318		22	1	0.12824	4.273318	-1.20106
23	8	0.582066	4.181608	-2.25019		23	1	-0.87863	4.337954	-0.01242
24	1	-0.24073	4.654701	-2.45461		24	8	1.225807	4.790348	-2.70996
25	1	1.271839	4.567721	-2.84486		25	1	0.75671	5.155672	-3.47892
26	8	2.48262	5.264623	-3.91735		26	1	1.954534	5.407368	-2.52826
27	1	2.693946	4.972272	-4.81789		27	8	-1.71819	-0.73741	-0.90922
28	1	3.008256	6.064447	-3.75911		28	1	-1.7478	-1.42828	-0.22039
29	11	1.029989	1.364118	0.417622		29	1	-2.39866	-0.97741	-1.5564
Na4_f						**K4_f**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	-1.8159	-1.04025	2.502872		1	1	-0.72164	-1.10573	2.834197
2	6	-1.13739	-1.77636	2.079994		2	6	-0.07337	-1.70858	2.203529

3	6	0.632068	-3.75449	1.019515		3	6	1.631978	-3.34247	0.594611
4	6	0.241977	-1.50706	1.986052		4	6	1.203944	-1.242	1.837606
5	6	-1.61277	-3.01299	1.647071		5	6	-0.48068	-2.96936	1.769604
6	6	-0.73464	-3.99126	1.11905		6	6	0.365765	-3.7778	0.971396
7	6	1.105175	-2.51286	1.464359		7	6	2.039365	-2.0785	1.041328
8	1	1.305742	-4.51379	0.631665		8	1	2.285945	-3.97166	-0.00317
9	1	-2.66769	-3.25191	1.758891		9	1	-1.44274	-3.36251	2.089995
10	1	-1.13343	-4.9527	0.807991		10	1	0.02882	-4.765	0.667568
11	1	0.769611	0.511531	2.87009		11	1	1.668907	0.764251	2.778881
12	7	2.392684	-2.01446	1.51825		12	7	3.234512	-1.40999	0.862517
13	1	3.226786	-2.51858	1.251005		13	1	4.044316	-1.7784	0.383521
14	6	2.376775	-0.74862	2.062827		14	6	3.192296	-0.20214	1.530417
15	6	1.077361	-0.38925	2.352392		15	6	1.962268	-0.0518	2.130011
16	1	3.302413	-0.21695	2.239796		16	1	4.063409	0.439265	1.556099
17	8	-1.94108	-1.40269	-1.20911		17	19	0.775566	1.637286	-0.46085
18	1	-2.61945	-1.78266	-1.79093		18	8	-1.75155	-1.46154	-0.82328
19	1	-1.89497	-1.98211	-0.41917		19	1	-2.47444	-1.99175	-1.19641
20	8	0.69378	-0.61074	-1.75859		20	1	-1.3708	-1.992	-0.09064
21	1	1.251758	-0.99394	-2.45086		21	8	0.401372	-0.30203	-2.24329
22	1	-0.17997	-1.0542	-1.81013		22	1	0.712576	-0.67724	-3.08004
23	8	-1.51442	1.173964	-0.17249		23	1	-0.35348	-0.85531	-1.94961
24	1	-1.95739	0.395864	-0.57216		24	8	-1.78441	1.198988	0.136597
25	1	-2.18274	1.86796	-0.07422		25	1	-2.03776	0.299808	-0.16074
26	11	0.732443	0.910721	-0.08957		26	1	-2.59107	1.623819	0.463733
27	8	1.998272	2.803905	-0.3331		27	8	1.725272	4.116884	-1.10016
28	1	2.515017	3.31218	0.312292		28	1	2.194409	4.765761	-0.55145
29	1	2.038887	3.317082	-1.15628		29	1	1.593276	4.560702	-1.95357
Na4_g						**K4_g**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	-2.09614	0.316375	1.728856		1	1	-2.09013	0.280669	1.735759
2	6	-1.62493	0.028756	0.792503		2	6	-1.63029	-0.07398	0.816675
3	6	-0.43628	-0.74692	-1.68877		3	6	-0.47987	-1.04888	-1.61029
4	6	-0.55676	-0.89181	0.78381		4	6	-0.47028	-0.87373	0.862232
5	6	-2.08379	0.546766	-0.41855		5	6	-2.19607	0.228929	-0.4204
6	6	-1.4924	0.164584	-1.64802		6	6	-1.62422	-0.25158	-1.62289
7	6	0.014621	-1.273	-0.46904		7	6	0.080721	-1.35824	-0.36257
8	1	0.001085	-1.05312	-2.63553		8	1	-0.06073	-1.44023	-2.53388
9	1	-2.92383	1.235864	-0.42544		9	1	-3.1087	0.817423	-0.46501
10	1	-1.88233	0.571334	-2.57672		10	1	-2.10252	-0.02119	-2.571
11	1	-0.03707	-1.59801	2.868978		11	1	0.201716	-1.26273	2.987525
12	7	1.015646	-2.18211	-0.19864		12	7	1.177588	-2.1304	-0.03772
13	1	1.576011	-2.66193	-0.88919		13	1	1.749143	-2.64453	-0.6933
14	6	1.090736	-2.39109	1.164317		14	6	1.329941	-2.15811	1.334502
15	6	0.154519	-1.61399	1.804307		15	6	0.350599	-1.39366	1.923836

16	1	1.802164	-3.09726	1.570703		16	1	2.121872	-2.74106	1.785097
17	8	0.496665	3.783301	-1.29924		17	19	0.453476	2.141469	-0.59208
18	1	1.133973	4.49554	-1.13994		18	8	0.395204	4.511745	-1.77762
19	1	-0.12458	4.123369	-1.98547		19	1	0.99827	5.264707	-1.6847
20	8	1.954305	1.238271	1.215163		20	1	-0.29651	4.806048	-2.4134
21	1	1.847152	0.393034	1.683625		21	8	2.161722	1.369839	1.241363
22	1	2.743146	1.681564	1.601128		22	1	1.970371	0.511099	1.657874
23	8	-1.30652	4.632653	-3.21643		23	1	2.960738	1.722782	1.689432
24	1	-1.08988	4.726705	-4.15751		24	8	-1.62522	5.217326	-3.56169
25	1	-2.01821	5.267796	-3.03874		25	1	-1.49966	5.2901	-4.52094
26	11	0.417806	1.80365	-0.28412		26	1	-2.35841	5.812931	-3.34043
27	8	4.146515	2.597499	2.247058		27	8	4.422952	2.451622	2.501868
28	1	5.073628	2.428755	2.016916		28	1	5.352381	2.270226	2.292788
29	1	4.158459	3.043074	3.108675		29	1	4.421714	2.908142	3.357526

Na4_h						**K4_h**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.465116	-2.49054	0.574423		1	1	2.149381	-2.26682	0.702563
2	6	1.926953	-1.82455	1.243181		2	6	1.576653	-1.64882	1.38982
3	6	0.547895	-0.07464	3.034802		3	6	0.13503	-0.02665	3.247443
4	6	0.607364	-2.12393	1.640633		4	6	0.414728	-2.15194	2.006109
5	6	2.536199	-0.66924	1.73201		5	6	2.002883	-0.35946	1.704342
6	6	1.850162	0.20096	2.616704		6	6	1.286455	0.443803	2.624008
7	6	-0.05512	-1.24451	2.549991		7	6	-0.2827	-1.32652	2.934912
8	1	0.032903	0.583244	3.72963		8	1	-0.40375	0.586368	3.96501
9	1	3.563125	-0.44465	1.456557		9	1	2.923087	0.022838	1.269364
10	1	2.358469	1.081258	3.000385		10	1	1.654867	1.437313	2.864327
11	1	-0.11192	-4.0813	0.762268		11	1	0.011446	-4.30249	1.420317
12	7	-1.29881	-1.78252	2.802878		12	7	-1.34817	-2.06338	3.415534
13	1	-1.99112	-1.39131	3.426357		13	1	-2.00684	-1.75215	4.115529
14	6	-1.44266	-2.96128	2.099993		14	6	-1.3382	-3.31694	2.842385
15	6	-0.30516	-3.20306	1.36443		15	6	-0.28306	-3.41231	1.961615
16	1	-2.34226	-3.55323	2.203755		16	1	-2.07385	-4.05656	3.129192
17	8	-1.876	-1.6342	-1.29108		17	8	-2.17067	-2.71966	-0.59801
18	1	-2.59847	-2.01651	-1.84481		18	1	-2.90344	-3.35412	-0.62448
19	1	-1.70636	-2.27408	-0.57364		19	1	-1.7053	-2.89954	0.245416
20	8	0.60952	-0.6078	-1.95275		20	8	0.173926	-1.62349	-4.44467
21	1	1.113353	-0.7715	-2.76306		21	1	1.021311	-1.22373	-4.69813
22	1	-0.24535	-1.08833	-2.02682		22	1	0.068931	-2.38729	-5.03408
23	8	-1.59529	0.807251	-0.02236		23	8	0.209201	0.762228	-0.84014
24	1	-1.98775	0.054389	-0.52075		24	1	0.343465	1.722053	-0.81049
25	1	-2.22367	1.542972	-0.06138		25	1	0.681842	0.414248	-0.05798
26	11	0.625877	0.43976	0.031258		26	8	-3.412	0.484012	-3.58994
27	8	-3.89293	-2.76406	-2.80454		27	1	-3.46355	0.684892	-4.53808
28	1	-3.76137	-3.30259	-3.60064		28	1	-4.22259	0.857178	-3.20842

29	1	-4.82646	-2.50055	-2.80638		29	19	-1.366	-0.82012	-2.32476
Na5_a						**K5_a**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.395132	-2.08534	1.378047		1	1	4.381763	-1.53663	-9.014
2	6	1.660493	-1.48777	1.912275		2	6	3.647409	-2.01594	-8.37123
3	6	-0.22065	0.085812	3.376782		3	6	1.772091	-3.34253	-6.67265
4	6	0.418055	-2.04135	2.280275		4	6	2.444473	-2.51614	-8.91249
5	6	1.945782	-0.17218	2.274139		5	6	3.898584	-2.1772	-7.00966
6	6	1.011823	0.606972	2.998081		6	6	2.968351	-2.83225	-6.16763
7	6	-0.50017	-1.23891	3.016431		7	6	1.524774	-3.18258	-8.04401
8	1	-0.93028	0.68149	3.944793		8	1	1.074171	-3.8716	-6.02847
9	1	2.915473	0.253679	2.02871		9	1	4.836404	-1.82292	-6.59015
10	1	1.270188	1.624086	3.278847		10	1	3.203454	-2.96772	-5.1155
11	1	0.246191	-4.21526	1.666908		11	1	2.314773	-2.1709	-11.1433
12	7	-1.61072	-2.02088	3.271949		12	7	0.460963	-3.5945	-8.81984
13	1	-2.42145	-1.73146	3.800759		13	1	-0.31373	-4.1593	-8.50095
14	6	-1.42281	-3.27793	2.740143		14	6	0.685304	-3.23127	-10.1355
15	6	-0.19794	-3.33348	2.111266		15	6	1.87842	-2.56004	-10.2333
16	1	-2.17199	-4.04704	2.872251		16	1	-0.0301	-3.49281	-10.9033
17	8	-1.35688	-2.5987	-0.81734		17	8	2.056695	2.427831	-5.34915
18	1	-1.89534	-3.35676	-1.09104		18	1	2.018787	2.862687	-6.23281
19	1	-1.09914	-2.78118	0.110528		19	1	2.664116	2.943714	-4.79707
20	8	-0.02094	-1.38016	-4.19394		20	8	1.812271	2.764661	-8.05077
21	1	0.734707	-1.88587	-4.52814		21	1	2.228891	3.400597	-8.65231
22	1	-0.47864	-1.00261	-4.97122		22	1	0.928159	2.535756	-8.42352
23	8	0.594876	0.379781	-0.72989		23	8	-0.1477	0.925445	-4.79305
24	1	0.895707	1.295086	-0.83486		24	1	0.546862	1.619754	-4.70662
25	1	0.935352	0.092506	0.140803		25	1	-0.34147	0.600617	-3.89979
26	11	-0.75419	-0.82045	-2.0979		26	8	-2.20508	1.60047	-6.54823
27	8	-2.37221	0.402844	-3.16094		27	1	-1.63422	1.4563	-5.76145
28	1	-2.37839	0.418943	-4.1389		28	1	-2.84474	2.29499	-6.33082
29	1	-3.12794	0.931322	-2.86441		29	8	-0.4464	1.34274	-8.54796
30	8	-1.80371	0.023392	-5.94411		30	1	-1.20985	1.514822	-7.93196
31	1	-2.41671	-0.47282	-6.51221		31	1	-0.8287	1.11158	-9.40861
32	1	-1.48666	0.766435	-6.48458		32	19	1.515515	0.028274	-6.98053
Na5_b						**K5_b**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.379074	-1.84906	0.087736		1	1	2.40711	-2.35007	0.329414
2	6	1.796388	-1.33011	0.844979		2	6	1.858719	-1.73589	1.039292
3	6	0.313778	0.016833	2.882091		3	6	0.458581	-0.14123	2.951809
4	6	0.53739	-1.82507	1.240808		4	6	0.526702	-2.05095	1.375151
5	6	2.293879	-0.18099	1.45785		5	6	2.470425	-0.64507	1.652473

6	6	1.556499	0.488085	2.464549		6	6	1.775401	0.146889	2.597069
7	6	-0.17975	-1.14151	2.267093		7	6	-0.14945	-1.24624	2.339415
8	1	-0.24179	0.523437	3.666899		8	1	-0.06383	0.45466	3.695863
9	1	3.275167	0.194887	1.180386		9	1	3.506411	-0.41011	1.423249
10	1	1.97712	1.372344	2.934786		10	1	2.285656	0.97899	3.074475
11	1	-0.02761	-3.70049	0.104435		11	1	-0.20059	-3.90122	0.291592
12	7	-1.36129	-1.82789	2.46333		12	7	-1.41282	-1.78062	2.501952
13	1	-2.06816	-1.59659	3.147248		13	1	-2.11332	-1.44612	3.148598
14	6	-1.41537	-2.90723	1.606294		14	6	-1.55304	-2.88649	1.688998
15	6	-0.27817	-2.93887	0.831231		15	6	-0.39448	-3.08232	0.97205
16	1	-2.25889	-3.58394	1.629305		16	1	-2.46873	-3.46227	1.70059
17	8	2.016422	1.720245	-2.08059		17	19	0.530546	1.074149	-0.44028
18	1	2.585314	1.29237	-2.73682		18	8	2.285696	2.14569	-2.16421
19	1	2.063823	2.688477	-2.2424		19	1	3.004114	1.859545	-2.7472
20	8	-1.10466	-0.38778	-1.07408		20	1	2.196321	3.116429	-2.28551
21	1	-1.80912	-0.36604	-1.73936		21	8	-1.28391	-0.7787	-1.17277
22	1	-1.14086	-1.26988	-0.65649		22	1	-1.96923	-0.90622	-1.84623
23	8	0.028418	3.245221	-0.2114		23	1	-1.2697	-1.59874	-0.64156
24	1	0.519462	3.874848	-0.78466		24	8	-0.17121	3.666587	-0.37812
25	1	-0.5834	3.76689	0.327819		25	1	0.371997	4.241075	-0.96155
26	8	1.746369	4.5066	-2.02753		26	1	-0.82759	4.242529	0.04054
27	1	1.416478	5.021352	-2.80392		27	8	1.665705	4.896472	-2.13135
28	1	2.489357	5.016729	-1.66704		28	1	1.360413	5.354224	-2.9515
29	8	0.868485	5.975976	-4.18847		29	1	2.322959	5.485782	-1.72795
30	1	1.200809	5.919163	-5.09789		30	8	0.863902	6.234095	-4.40961
31	1	0.238422	6.713166	-4.17213		31	1	1.251101	6.15367	-5.29518
32	11	0.555636	1.055031	-0.47331		32	1	0.125352	6.857682	-4.48874
Na5_c						**K5_c**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	-1.48341	-0.27827	2.115466		1	1	-1.67481	-1.64446	2.264465
2	6	-0.8471	-1.0698	1.727128		2	6	-0.97942	-2.15869	1.605828
3	6	0.80476	-3.19221	0.761145		3	6	0.840711	-3.56729	-0.08795
4	6	0.542004	-0.87145	1.588		4	6	0.353909	-1.71648	1.486417
5	6	-1.39014	-2.30219	1.373478		5	6	-1.38462	-3.27953	0.885426
6	6	-0.57102	-3.3525	0.894037		6	6	-0.48146	-3.9772	0.047548
7	6	1.346112	-1.9495	1.114256		7	6	1.244082	-2.43876	0.638859
8	1	1.432022	-4.00534	0.405872		8	1	1.534413	-4.11318	-0.7219
9	1	-2.45641	-2.47368	1.493359		9	1	-2.40123	-3.64867	0.993329
10	1	-1.02347	-4.30736	0.642051		10	1	-0.82386	-4.8582	-0.48776
11	1	1.178349	1.1986	2.262075		11	1	0.772075	0.072288	2.812132
12	7	2.653017	-1.5006	1.086402		12	7	2.475643	-1.81215	0.712783
13	1	3.457008	-2.05701	0.831247		13	1	3.330585	-2.15665	0.298583
14	6	2.703761	-0.19537	1.528474		14	6	2.39944	-0.75085	1.597681
15	6	1.432766	0.235303	1.838052		15	6	1.116102	-0.64679	2.07991

16	1	3.650896	0.320687	1.608981		16	1	3.279068	-0.16427	1.82657
17	8	2.111686	1.975574	-2.15081		17	19	0.338528	0.821543	-0.7913
18	1	2.760064	1.679747	-2.80618		18	8	1.999004	1.872049	-2.62192
19	1	2.059563	2.95535	-2.21664		19	1	2.526192	1.592428	-3.3847
20	8	-0.76747	-0.59436	-1.52879		20	1	2.032958	2.854172	-2.60483
21	1	-1.15731	-0.8267	-2.38494		21	8	-1.68585	-0.81994	-1.42397
22	1	-1.07782	-1.26553	-0.89256		22	1	-2.37564	-0.92202	-2.09713
23	8	-0.15753	3.12745	-0.2788		23	1	-1.75551	-1.60461	-0.84773
24	1	0.296728	3.848077	-0.76955		24	8	0.097052	3.44125	-0.27475
25	1	-0.94	3.516641	0.138268		25	1	0.626228	4.020972	-0.86554
26	8	1.52573	4.69695	-1.87251		26	1	-0.40304	4.02761	0.311864
27	1	1.179582	5.239195	-2.62302		27	8	1.807295	4.647929	-2.16497
28	1	2.175013	5.256807	-1.41717		28	1	1.439522	5.247187	-2.85881
29	8	0.583334	6.238302	-3.95257		29	1	2.598891	5.092972	-1.82244
30	1	0.974103	6.31944	-4.83658		30	8	0.827599	6.365386	-4.09036
31	1	-0.14729	6.875216	-3.91626		31	1	1.054835	6.37491	-5.03316
32	11	0.602089	1.034978	-0.74062		32	1	0.191113	7.084473	-3.95442
Na5_d						**K5_d**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.338341	-1.64922	0.358572		1	1	2.578033	-1.87588	0.379667
2	6	1.747243	-1.36583	1.225416		2	6	1.999934	-1.28876	1.088096
3	6	0.244631	-0.64213	3.545099		3	6	0.519073	0.256266	2.981261
4	6	0.564527	-2.06264	1.542058		4	6	0.769773	-1.76891	1.578253
5	6	2.160352	-0.32723	2.058148		5	6	2.475849	-0.06326	1.546463
6	6	1.413025	0.032508	3.205858		6	6	1.740906	0.702853	2.482713
7	6	-0.16216	-1.68945	2.708744		7	6	0.053253	-0.98518	2.528087
8	1	-0.31724	-0.37557	4.436304		8	1	-0.03308	0.836539	3.715775
9	1	3.095333	0.188528	1.85065		9	1	3.442919	0.298454	1.206055
10	1	1.773256	0.830954	3.848788		10	1	2.152059	1.641775	2.84456
11	1	0.173585	-3.76236	0.095828		11	1	0.295996	-3.83592	0.782166
12	7	-1.24756	-2.5397	2.802791		12	7	-1.08084	-1.69569	2.872147
13	1	-1.92865	-2.54022	3.549314		13	1	-1.77219	-1.40403	3.548707
14	6	-1.22462	-3.43549	1.756103		14	6	-1.09828	-2.89409	2.192315
15	6	-0.1391	-3.17217	0.948057		15	6	0.008428	-2.97639	1.374571
16	1	-1.97308	-4.21333	1.683256		16	1	-1.88841	-3.61214	2.367712
17	8	-1.73685	-1.19746	-0.98406		17	19	0.475831	1.536533	-0.5828
18	1	-2.47965	-1.5632	-1.49125		18	8	-1.72977	-1.82619	-1.0827
19	1	-1.43091	-1.91162	-0.38082		19	1	-2.36608	-2.45494	-1.4601
20	8	0.620092	0.131482	-1.78463		20	1	-1.34167	-2.26435	-0.29265
21	1	0.954057	0.181342	-2.69226		21	8	0.401355	-0.46703	-2.37458
22	1	-0.19599	-0.41115	-1.80347		22	1	0.793448	-0.78862	-3.19962
23	8	-1.44377	1.183309	0.475087		23	1	-0.32109	-1.08675	-2.14308
24	1	-1.84299	0.419568	0.008247		24	8	-2.11566	0.871693	-0.31506
25	1	-2.16381	1.677144	0.89293		25	1	-2.24574	-0.05883	-0.59317

26	11	0.794675	1.324466	0.150454		26	1	-2.99681	1.255782	-0.19762
27	8	2.077744	3.168438	0.216544		27	8	1.466509	4.007391	-0.81582
28	1	2.264716	3.76971	0.952707		28	1	1.921636	4.571434	-0.1727
29	1	2.521815	3.560148	-0.57122		29	1	1.427716	4.537489	-1.64363
30	8	3.288875	4.160103	-2.07099		30	8	1.288777	5.471902	-3.18839
31	1	4.247292	4.137659	-2.22049		31	1	2.018318	5.630818	-3.80753
32	1	2.957104	4.928214	-2.56222		32	1	0.645611	6.181937	-3.34004
Na5_e						**K5_e**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.307368	-2.23854	0.463855		1	1	2.11365	-2.6111	0.780515
2	6	1.770263	-1.70948	1.246411		2	6	1.491897	-1.81005	1.172529
3	6	0.403761	-0.33666	3.346622		3	6	-0.0853	0.315164	2.248772
4	6	0.488182	-2.13507	1.645485		4	6	0.325773	-2.10327	1.904623
5	6	2.348188	-0.6145	1.888323		5	6	1.854994	-0.47707	0.98734
6	6	1.668564	0.067073	2.92771		6	6	1.071117	0.575206	1.519338
7	6	-0.16901	-1.4413	2.703295		7	6	-0.43923	-1.02666	2.439907
8	1	-0.10712	0.177211	4.156546		8	1	-0.67442	1.124289	2.672201
9	1	3.357766	-0.30858	1.622605		9	1	2.777322	-0.2395	0.462877
10	1	2.154126	0.900625	3.427854		10	1	1.391653	1.603627	1.377095
11	1	-0.18031	-3.97263	0.505082		11	1	0.030154	-4.33413	2.159257
12	7	-1.37937	-2.07111	2.91309		12	7	-1.49313	-1.58348	3.139016
13	1	-2.04914	-1.83038	3.630214		13	1	-2.18872	-1.06766	3.659432
14	6	-1.5013	-3.1365	2.044361		14	6	-1.41142	-2.95844	3.079103
15	6	-0.38599	-3.20561	1.240575		15	6	-0.32074	-3.32263	2.320355
16	1	-2.36971	-3.78034	2.085677		16	1	-2.12808	-3.57312	3.607358
17	8	-1.82878	-1.36931	-1.1205		17	8	-3.37579	0.178705	-3.17249
18	1	-2.6075	-1.68935	-1.63385		18	1	-4.21412	0.64047	-3.32042
19	1	-1.66182	-2.02981	-0.41886		19	1	-2.66118	0.764514	-3.50454
20	8	0.68191	-0.51729	-1.93013		20	8	-0.04953	-1.4976	-4.25929
21	1	1.083126	-0.73546	-2.78358		21	1	0.515888	-1.94619	-4.90725
22	1	-0.20792	-0.93686	-1.90388		22	1	0.485576	-1.3373	-3.45236
23	8	-1.26764	1.065882	0.056285		23	8	0.070723	-0.48578	-1.7717
24	1	-1.73282	0.298682	-0.34865		24	1	-0.09044	0.421188	-2.09794
25	1	-1.93722	1.637412	0.457806		25	1	0.563047	-0.41339	-0.93027
26	11	0.966227	0.820478	-0.11932		26	8	-2.28606	-3.72449	-0.27002
27	8	2.261638	2.685149	-0.42889		27	1	-1.77542	-3.575	0.553272
28	1	3.05119	2.991193	0.044944		28	1	-2.78999	-4.53778	-0.11139
29	1	2.088692	3.358235	-1.10635		29	19	-2.18137	-2.04315	-2.35592
30	8	-4.02067	-2.32979	-2.52469		30	8	-0.86699	1.156323	-3.90559
31	1	-3.96971	-2.8804	-3.32168		31	1	-0.5517	0.372857	-4.40757
32	1	-4.90858	-1.93938	-2.52192		32	1	-0.62041	1.944266	-4.41497
Na5_f						**K5_f**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		

		X	Y	Z				X	Y	Z
1	1	2.218155	-2.13692	0.760527		1	1	2.586591	-1.95291	0.491193
2	6	1.62433	-1.55573	1.461823		2	6	1.997704	-1.34188	1.169915
3	6	0.122407	-0.03625	3.358717		3	6	0.486697	0.267031	2.984333
4	6	0.432421	-2.08206	1.996814		4	6	0.748491	-1.7947	1.637517
5	6	2.049234	-0.2936	1.874607		5	6	2.476846	-0.1115	1.61158
6	6	1.302451	0.459264	2.813061		6	6	1.726925	0.686745	2.508348
7	6	-0.29501	-1.30865	2.94706		7	6	0.017301	-0.97953	2.549004
8	1	-0.43958	0.536707	4.091453		8	1	-0.07807	0.872201	3.68857
9	1	2.989711	0.105475	1.502781		9	1	3.456891	0.230643	1.288507
10	1	1.670327	1.431179	3.129975		10	1	2.139034	1.631001	2.854685
11	1	0.024752	-4.18048	1.246814		11	1	0.267536	-3.8727	0.875395
12	7	-1.38936	-2.05928	3.331025		12	7	-1.13502	-1.66696	2.878602
13	1	-2.07639	-1.78379	4.018749		13	1	-1.84134	-1.34965	3.527571
14	6	-1.37167	-3.27082	2.674415		14	6	-1.1507	-2.8806	2.225931
15	6	-0.28008	-3.32438	1.835275		15	6	-0.02349	-2.99652	1.441056
16	1	-2.13026	-4.01517	2.876522		16	1	-1.95507	-3.58393	2.396216
17	8	-1.93606	-2.22006	-0.71091		17	19	0.552269	1.45002	-0.59024
18	1	-2.71524	-2.77363	-0.87207		18	8	-1.70521	-1.87796	-1.07805
19	1	-1.53498	-2.55902	0.116699		19	1	-2.34398	-2.50455	-1.45488
20	8	0.782915	-0.55064	-3.21747		20	1	-1.34098	-2.30449	-0.27069
21	1	1.397597	0.023742	-2.73122		21	8	0.479716	-0.58444	-2.34552
22	1	1.260805	-0.89439	-3.98728		22	1	0.876671	-0.91566	-3.16442
23	8	0.337859	0.779835	-0.71716		23	1	-0.25896	-1.18796	-2.12309
24	1	0.205964	1.718475	-0.51027		24	8	-2.06038	0.844848	-0.37981
25	1	0.7755	0.402881	0.07426		25	1	-2.19917	-0.08889	-0.64257
26	11	-1.13489	-0.5261	-1.98296		26	1	-2.93747	1.247777	-0.30131
27	8	-2.76071	0.443483	-3.20007		27	8	1.578846	3.851814	-1.15006
28	1	-2.60648	0.942889	-4.01591		28	1	2.328315	4.276827	-0.67549
29	1	-3.73857	0.391365	-3.09742		29	1	1.33316	4.471693	-1.85328
30	8	-5.51536	0.233553	-2.87085		30	8	3.72098	4.954047	0.27231
31	1	-6.05248	0.930576	-2.46235		31	1	4.625644	4.984871	-0.07679
32	1	-6.09588	-0.21634	-3.50477		32	1	3.635008	5.719713	0.861818
Na5_g						**K5_g**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.374064	-1.9393	0.168016		1	1	2.304345	-2.23602	1.025113
2	6	1.78824	-1.3769	0.891096		2	6	1.644921	-1.61471	1.626118
3	6	0.301896	0.094029	2.83676		3	6	-0.03511	0.020055	3.258817
4	6	0.608014	-1.9242	1.433025		4	6	0.42049	-2.12227	2.102038
5	6	2.207281	-0.11696	1.316127		5	6	2.01363	-0.31452	1.96676
6	6	1.468021	0.612978	2.277965		6	6	1.179431	0.494893	2.774708
7	6	-0.11207	-1.17499	2.410833		7	6	-0.39658	-1.29035	2.920598
8	1	-0.25335	0.649451	3.588187		8	1	-0.66687	0.638683	3.890632
9	1	3.130583	0.303102	0.925815		9	1	2.975376	0.073573	1.640245

10	1	1.828045	1.585435	2.601599		10	1	1.502488	1.4984	3.037391
11	1	0.168081	-3.97921	0.592925		11	1	0.116072	-4.28636	1.507135
12	7	-1.20444	-1.93309	2.779588		12	7	-1.50638	-2.03264	3.276722
13	1	-1.88602	-1.67868	3.480482		13	1	-2.25373	-1.71659	3.878469
14	6	-1.19747	-3.1221	2.078376		14	6	-1.41176	-3.29509	2.731255
15	6	-0.11102	-3.15483	1.235785		15	6	-0.25287	-3.39193	1.992927
16	1	-1.96614	-3.86341	2.249968		16	1	-2.17149	-4.03804	2.934301
17	8	1.642817	1.347511	-2.32702		17	8	-1.81909	-2.75066	-0.79947
18	1	2.19544	0.869993	-2.96324		18	1	-2.45697	-3.46921	-0.92909
19	1	1.645446	2.287701	-2.59604		19	1	-1.44206	-2.90067	0.091832
20	8	-1.27567	-0.88726	-1.01975		20	8	-0.41487	-1.40061	-5.01396
21	1	-1.99922	-0.98979	-1.67559		21	1	-0.96979	-1.04299	-5.7352
22	1	-1.25241	-1.7095	-0.5002		22	1	0.291461	-1.91028	-5.43831
23	8	-3.31886	-1.16752	-2.91413		23	8	0.548409	0.630579	-0.87181
24	1	-3.25858	-1.71917	-3.70949		24	1	0.884485	1.538307	-0.92751
25	1	-4.26492	-1.03251	-2.74927		25	1	0.900397	0.281851	-0.02925
26	8	-0.36446	2.897668	-0.49756		26	8	-3.01992	0.506296	-3.94291
27	1	0.039632	3.53226	-1.12248		27	1	-2.95808	0.414235	-4.91458
28	1	-1.00193	3.393772	0.036783		28	1	-3.79421	1.062291	-3.76956
29	8	1.179237	4.165283	-2.55131		29	19	-1.11559	-0.7526	-2.47542
30	1	0.7476	4.54096	-3.33693		30	8	-2.36845	-0.0946	-6.69045
31	1	1.887965	4.78766	-2.31641		31	1	-2.98131	-0.63611	-7.2155
32	11	0.255473	0.700846	-0.622		32	1	-2.08141	0.62432	-7.27804
Na5_h						**K5_h**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	-1.43587	-0.76425	2.894723		1	1	2.47148	-2.25671	0.374775
2	6	-0.75746	-1.43691	2.37657		2	6	1.895052	-1.63346	1.053982
3	6	1.018883	-3.24737	1.060661		3	6	0.426306	-0.00587	2.884697
4	6	0.582886	-1.06714	2.152494		4	6	0.628851	-2.05515	1.506925
5	6	-1.19288	-2.68806	1.942424		5	6	2.408353	-0.42179	1.510934
6	6	-0.31136	-3.58351	1.288306		6	6	1.679006	0.386152	2.415114
7	6	1.452038	-1.99088	1.504316		7	6	-0.08221	-1.23006	2.428623
8	1	1.697003	-3.94271	0.573278		8	1	-0.12014	0.605414	3.598507
9	1	-2.21339	-3.00277	2.146879		9	1	3.395498	-0.10016	1.189654
10	1	-0.67607	-4.55863	0.978031		10	1	2.114104	1.316288	2.77042
11	1	1.057514	0.959711	3.043784		11	1	0.05881	-4.07363	0.65725
12	7	2.700036	-1.40255	1.442534		12	7	-1.26401	-1.8781	2.727097
13	1	3.53111	-1.83211	1.061048		13	1	-1.96236	-1.55438	3.381178
14	6	2.654234	-0.15724	2.032214		14	6	-1.31897	-3.07406	2.039023
15	6	1.372805	0.095903	2.471078		15	6	-0.18621	-3.2181	1.272726
16	1	3.551328	0.440909	2.121469		16	1	-2.16175	-3.74008	2.165994
17	8	-1.81438	-0.90339	-0.75814		17	19	0.16713	0.814116	-0.60709
18	1	-2.52098	-1.29868	-1.29409		18	8	1.81996	1.783317	-2.52258
19	1	-1.66563	-1.51213	-0.0031		19	1	2.47333	1.41266	-3.13447

20	8	0.699483	0.09521	-1.52739		20	1	1.776653	2.741706	-2.71112
21	1	1.1463	-0.13637	-2.35439		21	8	-1.53055	-1.17337	-1.0442
22	1	-0.14325	-0.40642	-1.50163		22	1	-2.25489	-1.38096	-1.67157
23	8	-1.45118	1.655005	0.360048		23	1	-1.43347	-1.95556	-0.47287
24	1	-1.8666	0.857464	-0.03083		24	8	-3.59816	-1.75061	-2.87511
25	1	-2.15593	2.302212	0.509044		25	1	-3.50539	-2.28438	-3.67933
26	11	0.813822	1.618378	0.147725		26	1	-4.5504	-1.62893	-2.73875
27	8	2.041552	3.504826	0.174747		27	8	-0.44741	3.456091	-0.63035
28	1	2.168957	4.143859	0.891769		28	1	0.046666	4.013017	-1.26449
29	1	2.449249	3.914209	-0.6239		29	1	-1.07023	4.044474	-0.17812
30	8	3.150421	4.568669	-2.13043		30	8	1.275037	4.61323	-2.63835
31	1	4.1029	4.660043	-2.29059		31	1	0.882836	4.991661	-3.44298
32	1	2.719752	5.254843	-2.66429		32	1	1.968316	5.236452	-2.36364
Na5_i						**K5_i**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.165004	-2.25523	0.68783		1	1	-1.7665	-1.02586	2.763122
2	6	1.599674	-1.66393	1.404079		2	6	-0.92333	-1.54303	2.312418
3	6	0.176955	-0.11779	3.339662		3	6	1.293549	-2.94709	1.18185
4	6	0.439983	-2.18836	2.006392		4	6	0.309779	-0.8848	2.14021
5	6	2.032573	-0.39066	1.7697		5	6	-1.03611	-2.87712	1.923229
6	6	1.325423	0.375214	2.727466		6	6	0.0638	-3.57136	1.361819
7	6	-0.24819	-1.40147	2.974805		7	6	1.403088	-1.60871	1.581684
8	1	-0.35326	0.464968	4.088209		8	1	2.140265	-3.4869	0.766315
9	1	2.95056	0.007621	1.34459		9	1	-1.96727	-3.41092	2.09869
10	1	1.699683	1.356141	3.006923		10	1	-0.04928	-4.61653	1.087619
11	1	0.018949	-4.30792	1.325355		11	1	0.257353	1.226731	2.954434
12	7	-1.31497	-2.15383	3.428264		12	7	2.487959	-0.75489	1.557701
13	1	-1.97029	-1.87009	4.143072		13	1	3.421898	-1.00475	1.264541
14	6	-1.31689	-3.37919	2.798008		14	6	2.12699	0.464898	2.09672
15	6	-0.26739	-3.44075	1.906922		15	6	0.798503	0.433607	2.453807
16	1	-2.0567	-4.12613	3.053297		16	1	2.861676	1.250715	2.212939
17	8	-2.06636	-2.38758	-0.52991		17	19	0.029588	1.810012	-0.50694
18	1	-2.78774	-3.00439	-0.72773		18	8	-2.00701	-1.66746	-0.95034
19	1	-1.63567	-2.73078	0.282379		19	1	-2.5747	-2.31999	-1.39147
20	8	0.486438	-0.27094	-3.2098		20	1	-1.71383	-2.08146	-0.11021
21	1	0.899881	0.28436	-2.51836		21	8	0.232719	-0.34771	-2.07244
22	1	1.201471	-0.67867	-3.72154		22	1	0.731895	-0.75023	-2.79792
23	8	0.175446	0.836741	-0.70299		23	1	-0.49571	-0.96703	-1.85441
24	1	0.025833	1.803272	-0.5854		24	8	-2.52943	1.047834	-0.33343
25	1	0.667241	0.542543	0.088465		25	1	-2.60734	0.098034	-0.5625
26	11	-1.31933	-0.62915	-1.71442		26	1	-3.43034	1.380152	-0.20725
27	8	-2.27521	0.282079	-3.5456		27	8	0.939318	4.314935	-0.69386
28	1	-1.49805	0.421647	-4.11427		28	1	0.945415	5.046073	-0.05795
29	1	-3.05153	0.591564	-4.03553		29	1	1.270932	4.698964	-1.53706

30	8	-0.24418	3.576905	-0.489		30	8	1.843187	5.284053	-3.15061
31	1	0.379765	4.255456	-0.79065		31	1	2.765635	5.501442	-3.35759
32	1	-0.91094	4.038295	0.042996		32	1	1.299361	5.821791	-3.74745
Na5_j						**K5_j**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.298415	-2.13352	0.908249		1	1	-1.572	0.687218	2.912316
2	6	1.645319	-1.53026	1.534293		2	6	-1.17722	-0.26081	2.554301
3	6	-0.01025	0.055135	3.239237		3	6	-0.15596	-2.78275	1.686919
4	6	0.466141	-2.07935	2.074831		4	6	0.19652	-0.4001	2.264514
5	6	1.982364	-0.21338	1.846495		5	6	-2.01356	-1.36126	2.405412
6	6	1.159919	0.571614	2.690973		6	6	-1.50828	-2.61032	1.974857
7	6	-0.33987	-1.27065	2.928313		7	6	0.683081	-1.67008	1.836517
8	1	-0.63011	0.654208	3.90111		8	1	0.233137	-3.74937	1.377208
9	1	2.912517	0.206728	1.471888		9	1	-3.07045	-1.26959	2.639039
10	1	1.460855	1.58692	2.934133		10	1	-2.18301	-3.45818	1.892469
11	1	0.205214	-4.25291	1.496805		11	1	1.341965	1.518383	2.639819
12	7	-1.40378	-2.04856	3.34026		12	7	2.044349	-1.53867	1.635337
13	1	-2.129	-1.75791	3.980816		13	1	2.673745	-2.28804	1.384504
14	6	-1.2906	-3.31047	2.795472		14	6	2.431289	-0.24692	1.933265
15	6	-0.1662	-3.37149	2.003569		15	6	1.331031	0.486904	2.311646
16	1	-2.01544	-4.07715	3.033976		16	1	3.47172	0.041961	1.869817
17	8	-1.85141	-2.70505	-0.75269		17	19	-0.0256	0.97632	-0.71743
18	1	-2.44022	-3.44664	-1.01423		18	8	1.548389	2.327986	-2.45932
19	1	-1.4961	-2.93614	0.126991		19	1	2.263302	2.116661	-3.07812
20	8	0.365637	-0.24229	-3.42344		20	1	1.358152	3.280561	-2.57265
21	1	0.887637	0.246013	-2.75985		21	8	-1.22111	-1.30609	-1.30064
22	1	0.988788	-0.57083	-4.08975		22	1	-1.68191	-1.70824	-2.06759
23	8	0.176099	0.576566	-0.75038		23	1	-1.36985	-1.90702	-0.55063
24	1	-0.089	1.482904	-0.52556		24	8	-2.53885	-2.41911	-3.52575
25	1	0.697503	0.265955	0.020454		25	1	-2.18973	-3.11689	-4.10152
26	11	-1.30019	-0.87601	-1.8737		26	1	-3.49388	-2.38469	-3.69039
27	8	-2.36411	0.588972	-3.24494		27	8	-1.02915	3.48783	-0.57334
28	1	-1.69655	0.791819	-3.92228		28	1	-0.60713	4.166625	-1.13678
29	1	-3.20416	0.963641	-3.55005		29	1	-1.77129	3.924225	-0.1288
30	8	-3.51988	-4.78927	-1.57591		30	8	0.56699	5.041686	-2.40449
31	1	-4.47309	-4.87772	-1.42093		31	1	0.148576	5.408945	-3.2011
32	1	-3.23979	-5.60403	-2.02121		32	1	1.137965	5.747099	-2.05671
Na5_k						**K5_k**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	-1.06623	-0.85388	2.540863		1	1	1.82455	-2.88152	0.431186
2	6	-0.36484	-1.52726	2.054267		2	6	1.514857	-2.14108	1.164658
3	6	1.476613	-3.33508	0.828726		3	6	0.765161	-0.21447	3.136827

4	6	0.896267	-1.06334	1.626693		4	6	0.332863	-2.32222	1.908608
5	6	-0.69144	-2.86548	1.85715		5	6	2.301563	-1.01682	1.411494
6	6	0.22091	-3.75982	1.248865		6	6	1.927519	-0.06146	2.387691
7	6	1.800349	-1.98646	1.026928		7	6	-0.01523	-1.35187	2.892424
8	1	2.179689	-4.02732	0.373212		8	1	0.489655	0.510884	3.897737
9	1	-1.65325	-3.23948	2.197452		9	1	3.240961	-0.89114	0.878539
10	1	-0.06004	-4.8013	1.121285		10	1	2.572728	0.793069	2.572288
11	1	1.202204	1.132897	2.103649		11	1	-0.69286	-4.2763	1.400365
12	7	2.952365	-1.28648	0.717167		12	7	-1.18059	-1.78287	3.495863
13	1	3.790132	-1.687	0.318979		13	1	-1.65355	-1.31566	4.256568
14	6	2.812369	0.029493	1.104518		14	6	-1.56731	-2.98632	2.945147
15	6	1.563966	0.214997	1.657009		15	6	-0.67679	-3.349	1.958798
16	1	3.627465	0.729075	0.977559		16	1	-2.43896	-3.50564	3.320616
17	8	1.475354	1.760443	-2.433		17	8	-2.63634	-2.09364	-0.34486
18	1	1.944676	1.415461	-3.20701		18	1	-3.51721	-2.48558	-0.24204
19	1	1.378717	2.724988	-2.56531		19	1	-2.11718	-2.42441	0.41665
20	8	-1.11579	-0.9262	-1.12216		20	8	0.695425	-0.72319	-3.48764
21	1	-1.74572	-1.18224	-1.8311		21	1	1.176029	-0.26528	-2.77101
22	1	-1.16997	-1.61604	-0.43858		22	1	1.339682	-0.95478	-4.17245
23	8	-2.90273	-1.60155	-3.16232		23	8	0.713896	0.522115	-0.99928
24	1	-2.75798	-2.31892	-3.79882		24	1	0.925179	1.452938	-0.82329
25	1	-3.86384	-1.48912	-3.09661		25	1	1.085853	0.029059	-0.23844
26	8	-0.53277	2.897767	-0.26768		26	8	-3.48623	0.911357	-3.65731
27	1	-0.22767	3.637577	-0.8302		27	1	-3.34259	1.410026	-4.4758
28	1	-1.25741	3.23881	0.27748		28	1	-4.4484	0.989061	-3.46859
29	8	0.788536	4.532732	-2.21353		29	19	-1.67834	-0.5005	-2.29341
30	1	0.292184	4.993219	-2.91094		30	8	-6.2139	1.062039	-3.05082
31	1	1.464837	5.162611	-1.91201		31	1	-6.63206	1.847019	-2.66349
32	11	0.250787	0.800766	-0.75708		32	1	-6.90017	0.625414	-3.57953
Na5_l						**K5_l**				
Center Number	Atomic Number	Coordinates (Angstroms)				Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z				X	Y	Z
1	1	2.069072	1.640719	-0.34499		1	1	2.586591	-1.95291	0.491193
2	6	1.311372	1.452397	0.411469		2	6	1.997704	-1.34188	1.169915
3	6	-0.67403	1.005916	2.416541		3	6	0.486697	0.267031	2.984333
4	6	1.474287	0.403464	1.339343		4	6	0.748491	-1.7947	1.637517
5	6	0.17521	2.25581	0.489897		5	6	2.476846	-0.1115	1.61158
6	6	-0.8097	2.03215	1.482912		6	6	1.726925	0.686745	2.508348
7	6	0.473678	0.205242	2.337215		7	6	0.017301	-0.97953	2.549004
8	1	-1.42697	0.843874	3.183142		8	1	-0.07807	0.872201	3.68857
9	1	0.04537	3.076282	-0.21048		9	1	3.456891	0.230643	1.288507
10	1	-1.67814	2.683208	1.529718		10	1	2.139034	1.631001	2.854685
11	1	3.412609	-0.72004	1.012455		11	1	0.267536	-3.8727	0.875395
12	7	0.876243	-0.86608	3.1092		12	7	-1.13502	-1.66696	2.878602
13	1	0.388474	-1.22118	3.919702		13	1	-1.84134	-1.34965	3.527571

14	6	2.084925	-1.3407	2.643349		14	6	-1.1507	-2.8806	2.225931
15	6	2.48334	-0.60062	1.554049		15	6	-0.02349	-2.99652	1.441056
16	1	2.577405	-2.16576	3.140045		16	1	-1.95507	-3.58393	2.396216
17	8	-1.90752	0.982679	-2.33634		17	19	0.552269	1.45002	-0.59024
18	1	-1.82073	1.944301	-2.52892		18	8	-1.70521	-1.87796	-1.07805
19	1	-2.52389	0.630719	-2.99555		19	1	-2.34398	-2.50455	-1.45488
20	8	0.355765	-2.00089	-0.65565		20	1	-1.34098	-2.30449	-0.27069
21	1	0.681785	-2.51557	-1.42848		21	8	0.479716	-0.58444	-2.34552
22	1	1.112482	-1.91775	-0.04627		22	1	0.876671	-0.91566	-3.16442
23	8	1.231514	-3.48899	-2.84279		23	1	-0.25896	-1.18796	-2.12309
24	1	1.704973	-3.1691	-3.62641		24	8	-2.06038	0.844848	-0.37981
25	1	1.257324	-4.45756	-2.88659		25	1	-2.19917	-0.08889	-0.64257
26	8	-2.25239	-1.87209	0.210553		26	1	-2.93747	1.247777	-0.30131
27	1	-3.06683	-2.34624	0.433055		27	8	1.578846	3.851814	-1.15006
28	1	-1.54345	-2.5301	0.087226		28	1	2.328315	4.276827	-0.67549
29	8	-1.59231	3.720336	-2.75234		29	1	1.33316	4.471693	-1.85328
30	1	-2.30882	4.355928	-2.59619		30	8	3.72098	4.954047	0.27231
31	1	-1.06494	4.08682	-3.47979		31	1	4.625644	4.984871	-0.07679
32	11	-1.0461	-0.10719	-0.56909		32	1	3.635008	5.719713	0.861818
						k5_m				
						Center Number	Atomic Number	Coordinates (Angstroms)		
								X	Y	Z
						1	1	1.994855	-2.8777	0.580303
						2	6	1.561507	-2.12007	1.228528
						3	6	0.474087	-0.13397	2.969228
						4	6	0.367842	-2.37798	1.930151
						5	6	2.194069	-0.89334	1.402756
						6	6	1.655083	0.09101	2.264363
						7	6	-0.15361	-1.37318	2.79532
						8	1	0.071819	0.617379	3.643763
						9	1	3.128454	-0.69173	0.886025
						10	1	2.188255	1.028012	2.404026
						11	1	-0.39354	-4.47861	1.556875
						12	7	-1.30024	-1.88637	3.373173
						13	1	-1.87463	-1.413	4.056091
						14	6	-1.51027	-3.17005	2.918648
						15	6	-0.51981	-3.50971	2.023105
						16	1	-2.3424	-3.75367	3.289252
						17	8	-2.19556	-2.55071	-0.58254
						18	1	-3.02946	-3.04144	-0.64301
						19	1	-1.79491	-2.82287	0.268892
						20	8	0.38171	-1.95529	-4.04187
						21	1	1.12269	-1.61354	-4.56702
						22	1	0.337795	-2.90182	-4.25122
						23	8	0.162431	1.171624	-0.65167

						24	1	0.299789	2.14004	-0.72209
						25	1	0.61029	0.89772	0.168175
						26	8	-3.01749	0.431122	-3.76357
						27	1	-3.15228	0.222002	-4.70147
						28	1	-3.66914	1.120776	-3.56071
						29	19	-1.08757	-0.63346	-2.12673
						30	8	0.546742	3.955381	-0.92936
						31	1	1.339905	4.369387	-1.30341
						32	1	0.079296	4.65472	-0.44695