Impact of Long-Range van der Waals Forces on Chiral Recognition in a Cinchona Alkaloid Chiral Selector System

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Electronic Supplementary Information

Contents

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† Electronic Supplementary Information (ESI) available: Comparison of different functionals and basis sets, NBO charges and xyz coordinates of the all optimized structures are posted. See DOI: 10.1039/b000000x/
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1. The NCI Plots and the Optimized Structures

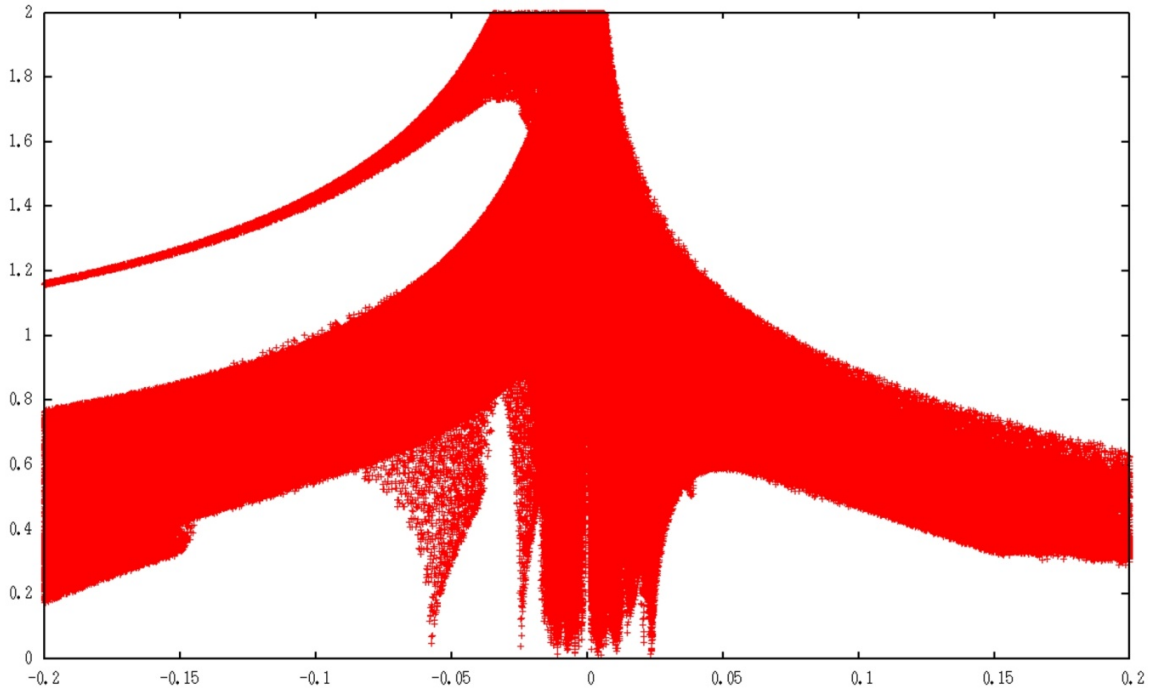

Fig. S1 Dependence of the reduced density gradient on the electron density multiplied by the sign of the second Hessian eigenvalue, so called NCIplot for $2_S Na^+$.

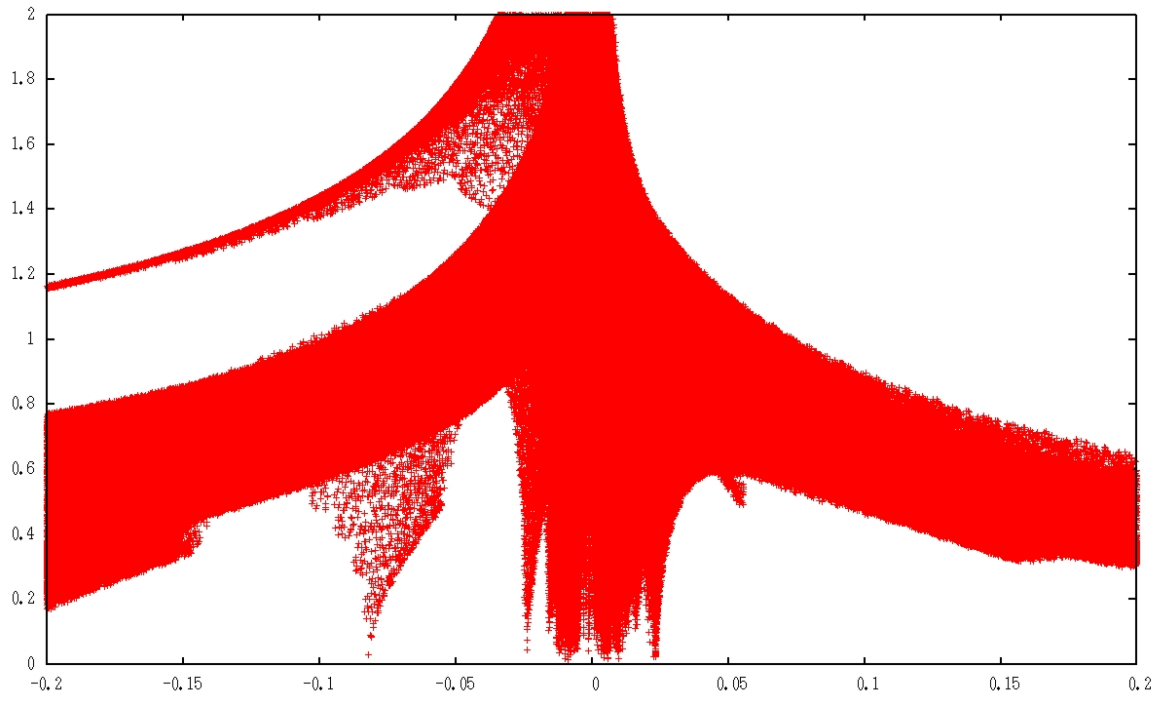

Fig. S2 Dependence of the reduced density gradient on the electron density multiplied by the sign of the second Hessian eigenvalue, so called NCIplot for $3_S Na^+$.

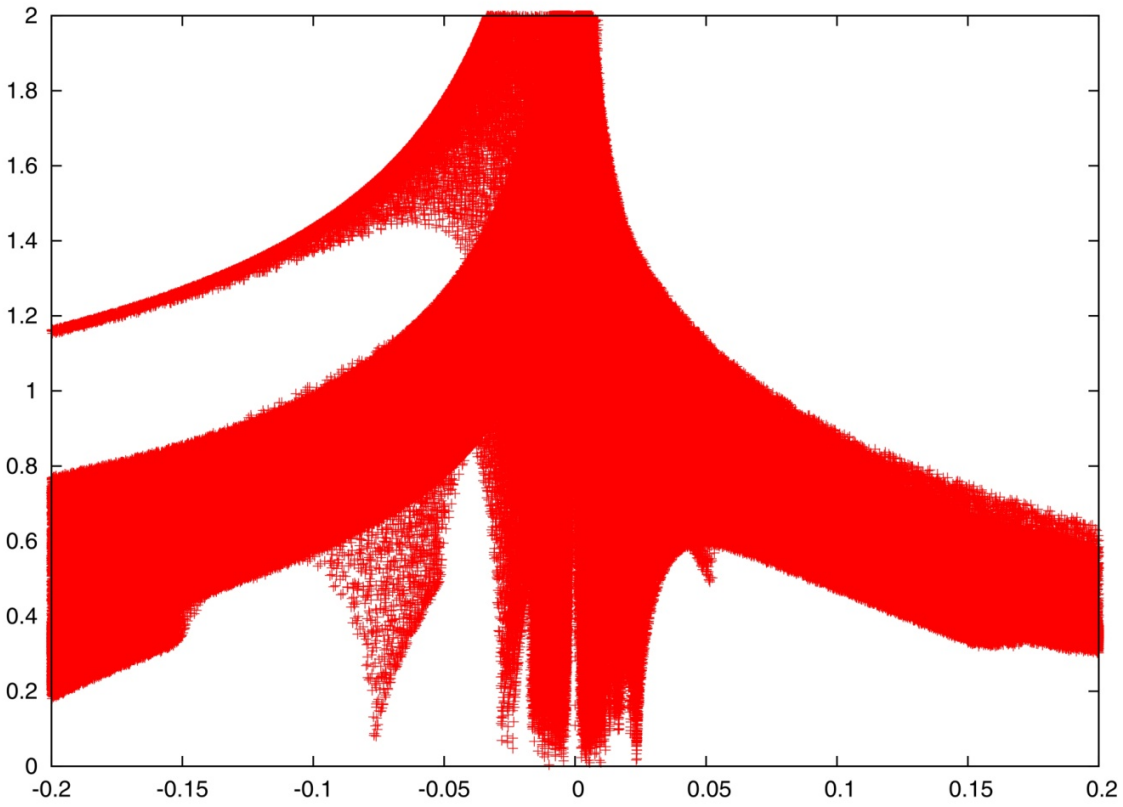

Fig. S3 Dependence of the reduced density gradient on the electron density multiplied by the sign of the second Hessian eigenvalue, so called NCIplot for $1_R Na^+$.

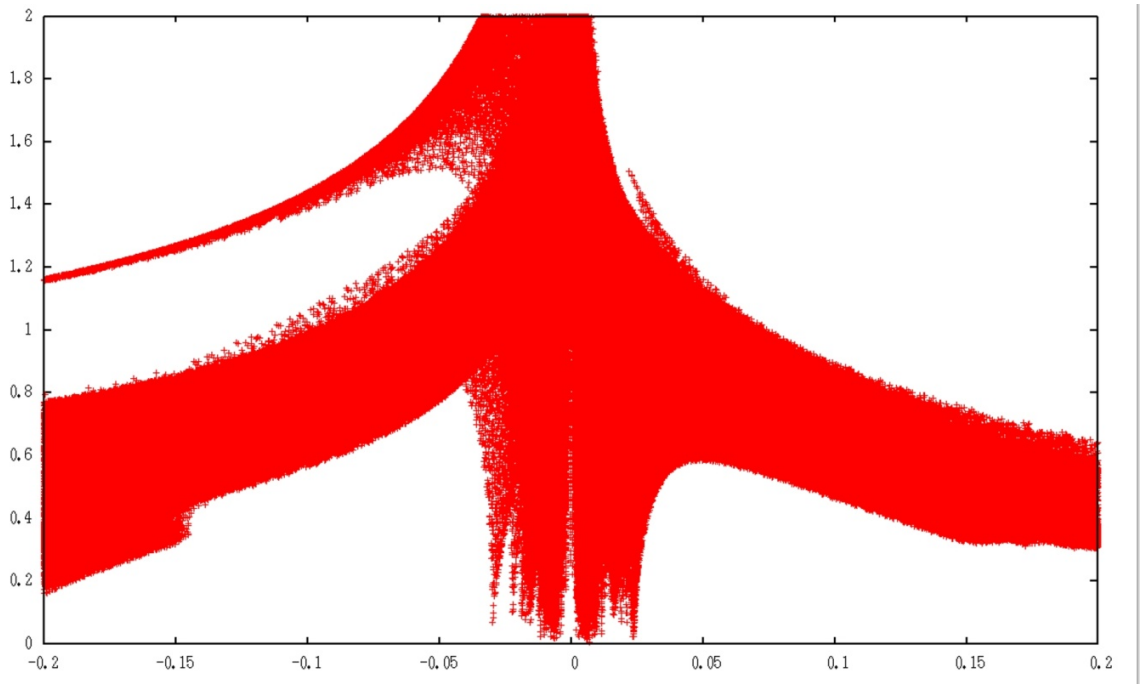

Fig. S4 Dependence of the reduced density gradient on the electron density multiplied by the sign of the second Hessian eigenvalue, so called NCIplot for $2_R Na^+$.

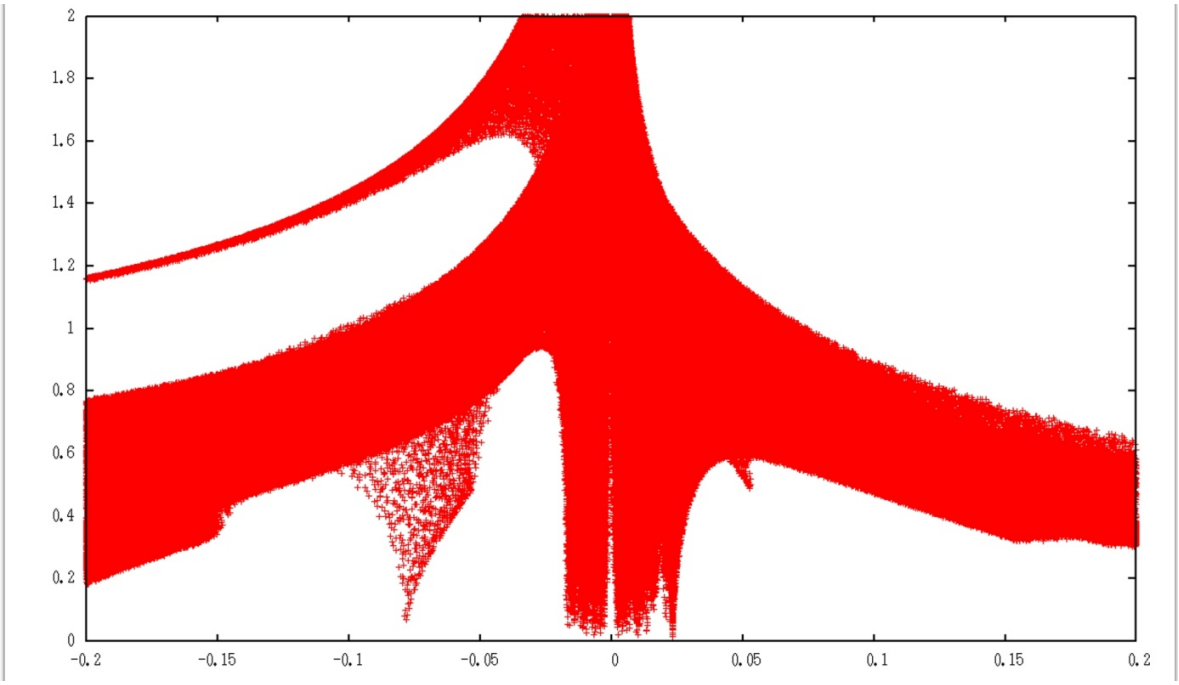

Fig. S5 Dependence of the reduced density gradient on the electron density multiplied by the sign of the second Hessian eigenvalue, so called NCIplot for $3_R Na^+$.

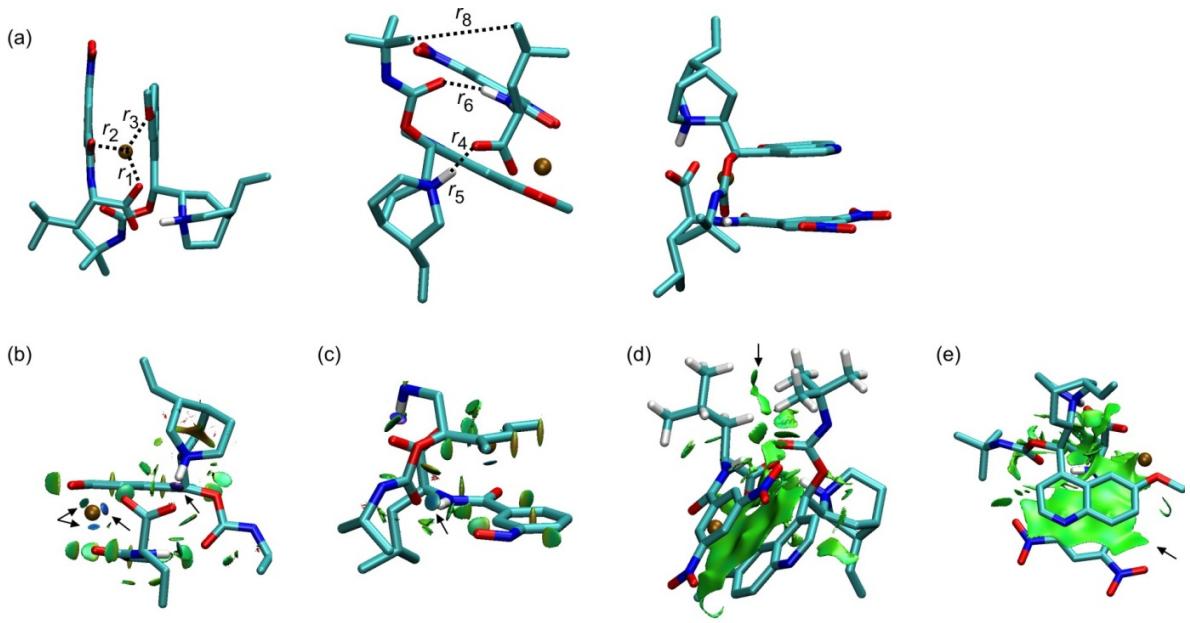

Fig. S6 The optimized structures of the $1_S Li^+$ complex (B97D/6-311++G**/DFBS). Hydrogen atoms were removed except of important ones to improve the clarity of the pictures. Colour codes: light blue, white, red, blue, and brown correspond to carbon, hydrogen, oxygen, nitrogen, and lithium, respectively. Colour codes of the isosurfaces: the weak-, the strong attractive-, and the strong repulsive interactios are in green, blue, and red, respectively. The black arrows indicate the isosurfaces discussed in the text.

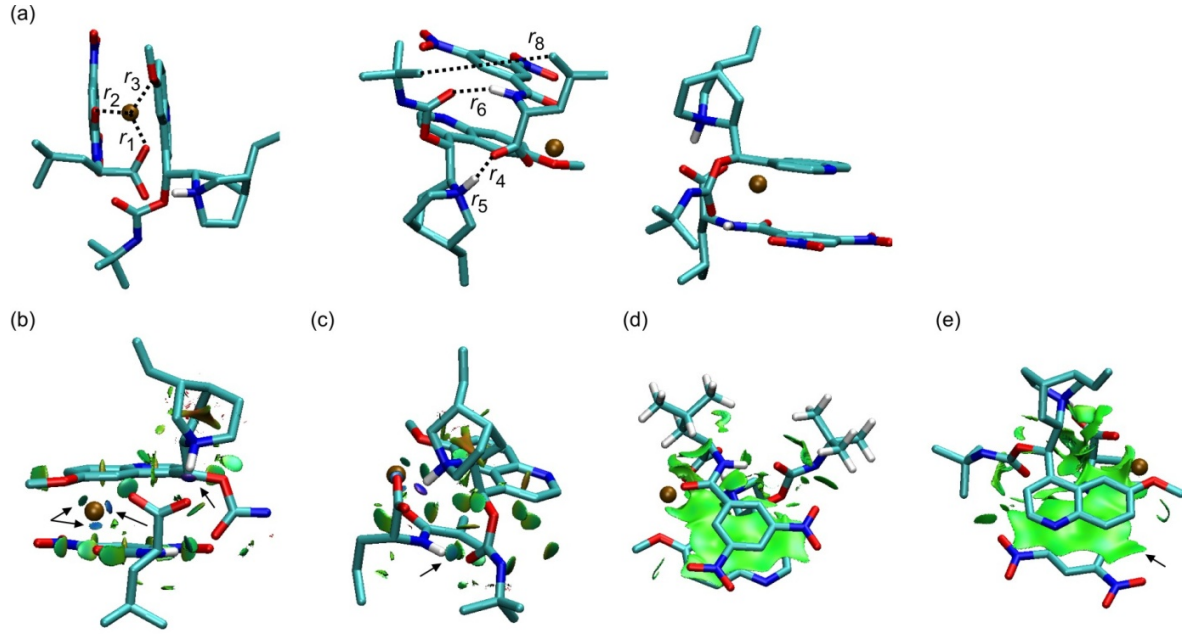

Fig. S7 The optimized structures of the $1_R Li^+$ complex (B97D/6-311++G**/DFBS). Hydrogen atoms were removed except of important ones to improve the clarity of the pictures. Colour codes: light blue, white, red, blue, and brown correspond to carbon, hydrogen, oxygen, nitrogen, and lithium, respectively. Colour codes of the isosurfaces: the weak-, the strong attractive-, and the strong repulsive interactios are in green, blue, and red, respectively. The black arrows indicate the isosurfaces discussed in the text.

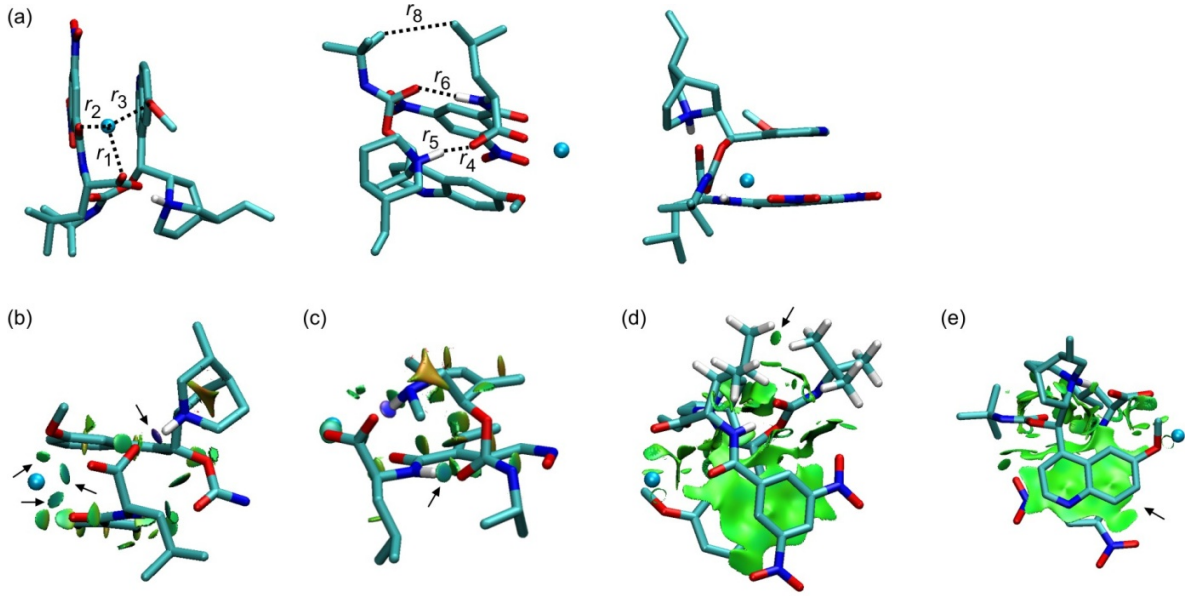

Fig. S8 The optimized structures of the $1_S K^+$ complex (B97D/6-311++G**/DFBS). Hydrogen atoms were removed except of the important ones to improve the clarity of the pictures. Colour codes: light blue, white, red, blue, and cyan correspond to carbon, hydrogen, oxygen, nitrogen, and potassium, respectively. Colour codes of the isosurfaces: the weak-, the strong attractive-, and the strong repulsive interactios are in green, blue, and red, respectively. The black arrows indicate the isosurfaces discussed in the text.

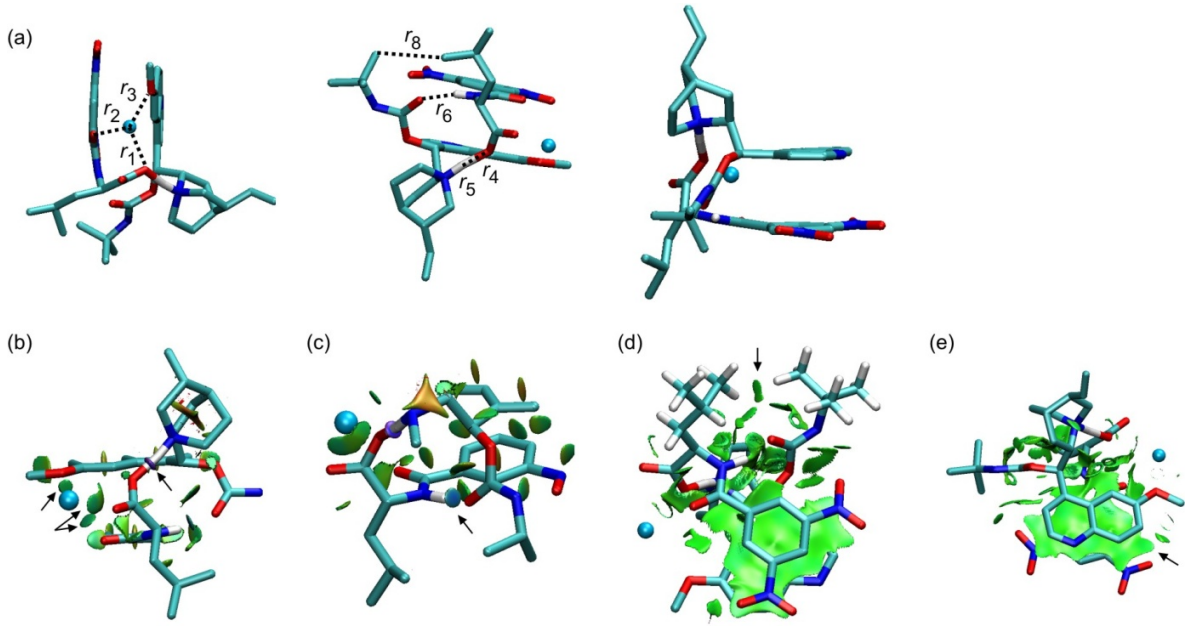

Fig. S9 The optimized structures of the 1_RK^+ complex (B97D/6-311++G**/DFBS). Hydrogen atoms were removed except of the important ones to improve the clarity of the pictures. Colour codes: light blue, white, red, blue, and cyan correspond to carbon, hydrogen, oxygen, nitrogen, and potassium, respectively. Colour codes of the isosurfaces: the weak-, the strong attractive-, and the strong repulsive interactios are in green, blue, and red, respectively. The black arrows indicate the isosurfaces discussed in the text.

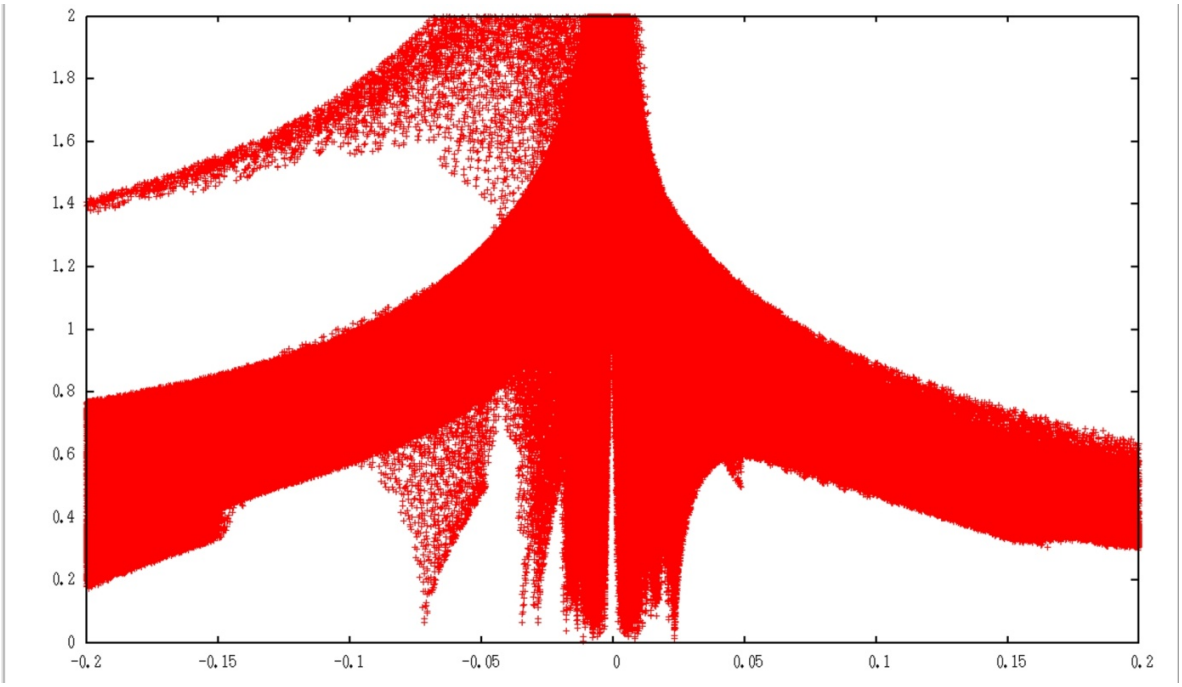

Fig. S10 Dependence of the reduced density gradient on the electron density multiplied by the sign of the second Hessian eigenvalue - so calledNCI plot for 1_SLi^+.

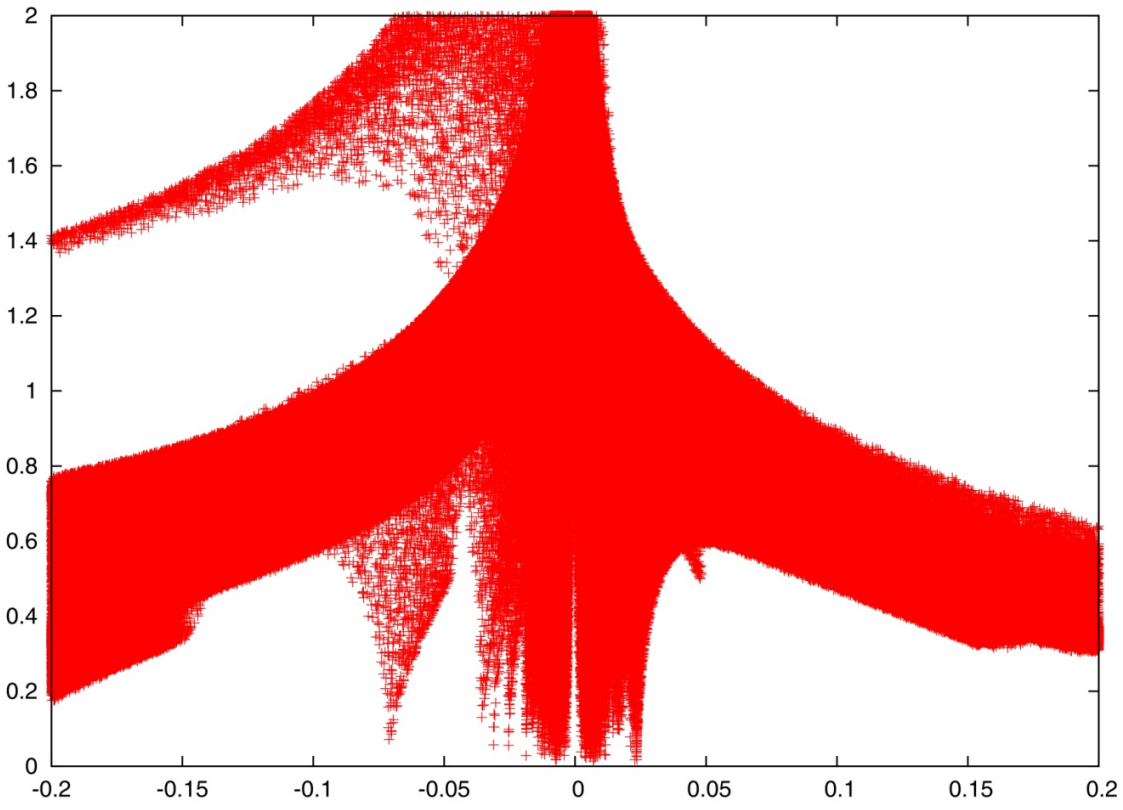

Fig. S11 Dependence of the reduced density gradient on the electron density multiplied by the sign of the second Hessian eigenvalue - so calledNCI plot for $1_R Li^+$.

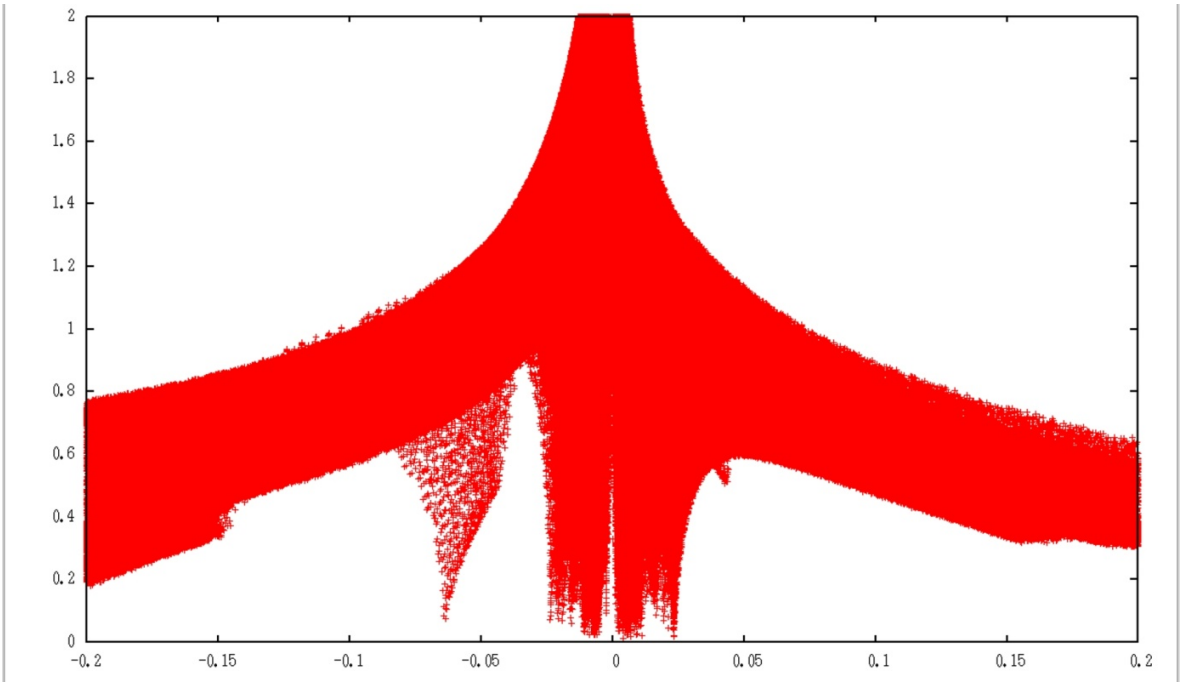

Fig. S12 Dependence of the reduced density gradient on the electron density multiplied by the sign of the second Hessian eigenvalue - so called NCIplot for $1_S K^+$.

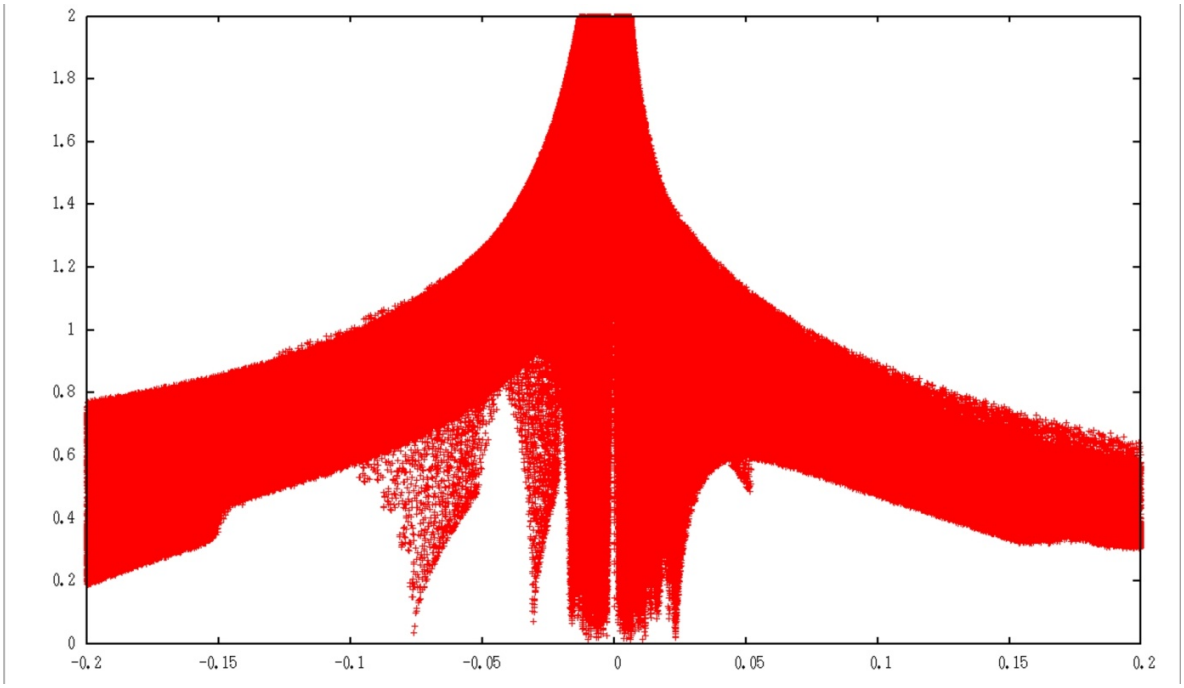

Fig. S13 Dependence of the reduced density gradient on the electron density multiplied by the sign of the second Hessian eigenvalue - so called NCIplot for 1_RK^+.

2. The NBO Analysis of the $1_S Na^+$ Isomer

The NBO analysis of $1_S Na^+$ isomer was done at the PBE0/6-311G**//B97D/6-311++G**/DFBS level of theory using the NBO program version 3.1 as is implemented in Gaussian 09.[S1,S2] Wiberg bond indexes (WBI) of about 1.4 of both C-O bonds in the carboxylate group demonstrate the π-electron delocalization over the COO^- group. In the main text, it is shown using the NCI plot that the $O^-(3)$–$H^+(4)$ ionic pair has a non-negligible covalent character. This agrees with a low value of WBI of the $O^-(3)$–$H^+(4)$ pair. The strong interaction of between $O^-(3)$ and $H^+(4)$ affects the $H^+(4)$–N(5) bond resulting in a low WBI of the $H^+(4)$–N(5) bond. One lone pair orbital of $O^-(3)$ is involved in the charge transfer to the σ* orbital of the $H^+(4)$–N(5) bond, while the second one is involved in the delocalization of the electrons over the COO^- moiety. In summary, the Lewis structure can be draw as the COO^- moiety with delocalized π-electrons that interacts with the σ* orbital of the $H^+(4)$–N(5) bond. This interaction has mostly Coulombic character however it has a slight covalent character in agreement with the NCI plot.

Table S1. The WBI's and NBO analysis of bonds involved in the $O^-(3)$–$H^+(4)$ ionic pair interaction.

	Na^+ – O(1)	O(1) – C(2)	C(2) – $O^-(3)$	$O^-(3)$ – $H^+(4)$	$H^+(4)$ – N(5)
WBI[a]	0.0687	1.4114	1.4361	0.1599	0.5634
occupancy of σ orbital	-	1.99512	1.99361		1.97472
occupancy of σ* orbital	-	0.04891	0.04936		0.12261

[a]Wiberg bond index

Table S2. Occupancies of lone pair orbitals of atoms involved in the $O^-(3)$–$H^+(4)$ ionic pair interaction.

	LP^1	LP^2	LP^3	LP^4
Na^+	0.04429	0.03127	0.02649	0.00872
O(1)	1.95246	1.89951	1.63069	-
$O^-(3)$	1.95928	1.83017	1.60514	-

3. The Relaxed Potential Energy Surface Scans

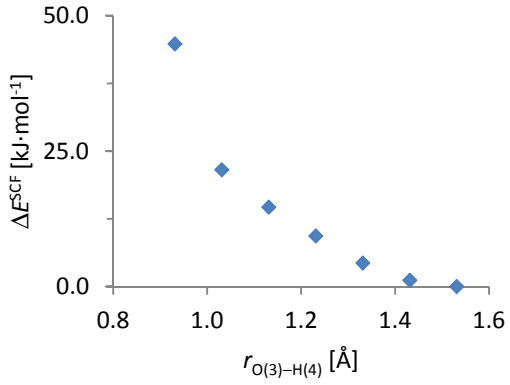

Fig. S14 The relaxed PES scan of the proton migration from N(5) to O-(3) in $1_S Na^+$ at the B97D/6-311++G**/DFBS level of theory.

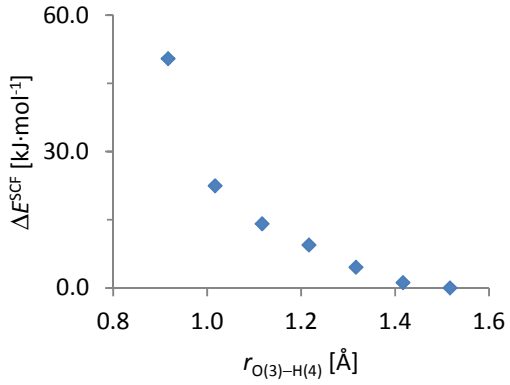

Fig. S15 The relaxed PES scan of the proton migration from N(5) to O-(3) in $1_R Na^+$ at the B97D/6-311++G**/DFBS level of theory.

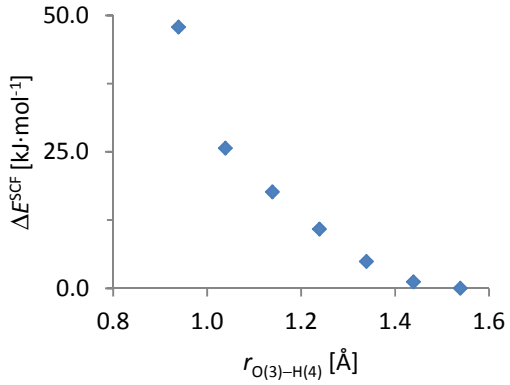

Fig. S16 The relaxed PES scan of the proton migration from N(5) to O^-(3) in $1_S Li^+$ at the B97D/6-311++G**/DFBS level of theory.

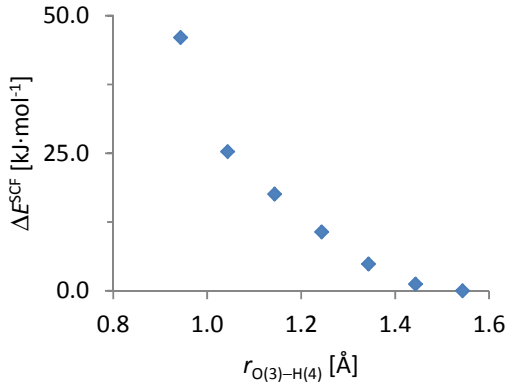

Fig. S17 The relaxed PES scan of the proton migration from N(5) to O^-(3) in $1_R Li^+$ at the B97D/6-311++G**/DFBS level of theory.

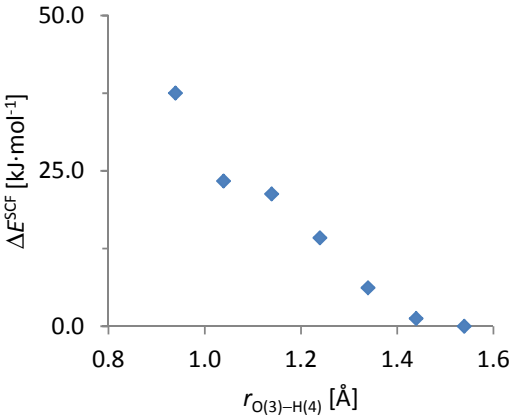

Fig. S18 The relaxed PES scan of the proton migration from N(5) to O^-(3) in $1_S K^+$ at the B97D/6-311++G**/DFBS level of theory.

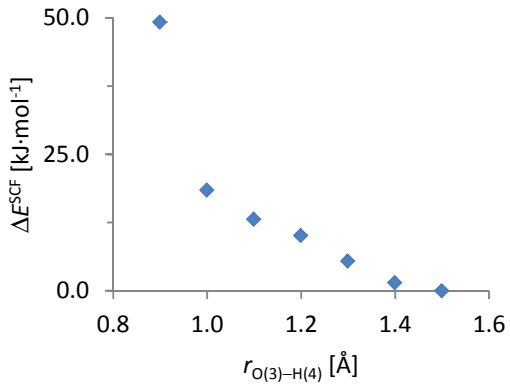

Fig. S19 The relaxed PES scan of the proton migration from N(5) to O^-(3) in $1_R K^+$ at the B97D/6-311++G**/DFBS level of theory.

4. Optimized Geometries (XYZ coordinates) of the Complexes

$1_S Na^+$

E(RB97D) = -2718.800758 A.U.
NImag = 0

Zero-point correction= 0.819918 (Hartree/Particle)
Thermal correction to Energy= 0.874789
Thermal correction to Enthalpy= 0.875733
Thermal correction to Gibbs Free Energy= 0.729673
Sum of electronic and zero-point Energies= -2717.980840
Sum of electronic and thermal Energies= -2717.925969
Sum of electronic and thermal Enthalpies= -2717.925025
Sum of electronic and thermal Free Energies= -2718.071085

E(RPBE1PBE) = -2717.44150274 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.140651	0.687712	-1.603809
2	6	0	-0.102331	0.194538	-2.894937
3	6	0	-1.616369	1.536484	0.267246
4	6	0	-1.411841	1.078633	-1.062883
5	6	0	1.138417	0.857282	-0.793601
6	6	0	-1.298236	0.093568	-3.653591
7	6	0	3.146398	-3.943134	-2.236577
8	6	0	2.508166	-1.108086	-1.109153
9	6	0	-2.885448	1.912904	0.693212
10	6	0	-2.550749	0.980308	-1.945153
11	6	0	4.162917	-2.934998	-1.669736
12	6	0	-3.996715	1.870563	-0.187945
13	6	0	-3.822680	1.404907	-1.476225
14	6	0	4.514360	-3.268540	-0.207224
15	6	0	5.439834	-2.923733	-2.527759
16	1	0	-0.788565	1.574719	0.973135
17	1	0	0.836582	-0.127738	-3.335995
18	1	0	2.218963	-3.930952	-1.655258
19	1	0	1.000369	0.422627	0.198337
20	1	0	2.909775	-3.708257	-3.282778
21	1	0	-1.262014	-0.320297	-4.662918
22	1	0	3.577400	-4.952159	-2.193670
23	1	0	3.613602	-3.288880	0.414462
24	1	0	4.038351	-0.905115	-2.406264
25	1	0	4.988574	-4.258049	-0.171208
26	1	0	5.207928	-2.666841	-3.571909
27	1	0	-4.985810	2.169496	0.143104
28	1	0	5.892500	-3.921937	-2.515546
29	1	0	-4.663745	1.335828	-2.162749
30	1	0	5.215939	-2.528205	0.200623
31	1	0	6.173595	-2.206851	-2.131717
32	7	0	-2.482860	0.483875	-3.215343
33	7	0	3.603868	-1.545862	-1.754396
34	8	0	1.808951	-1.756344	-0.338460
35	8	0	2.269062	0.225421	-1.425863
36	6	0	-4.301745	2.715600	2.498448
37	1	0	-4.658736	3.590656	1.939382
38	1	0	-5.020319	1.889318	2.411180
39	1	0	-4.158208	2.984984	3.549873
40	8	0	-2.996877	2.308995	2.016005
41	6	0	1.453110	2.354367	-0.622758
42	6	0	1.667640	3.168783	-1.916402
43	6	0	0.818625	5.588402	-0.287517
44	6	0	0.525807	6.892504	-0.230132
45	6	0	2.423337	3.995269	0.905153
46	6	0	2.221153	5.033349	-0.252066
47	6	0	2.631398	4.335379	-1.589231
48	6	0	3.968801	2.579433	-0.387908
49	6	0	4.048428	3.745055	-1.409903
50	1	0	0.595381	2.764566	-0.084973
51	1	0	0.005936	4.861719	-0.372848
52	1	0	0.697298	3.530567	-2.272499
53	1	0	-0.502766	7.248348	-0.271787
54	1	0	1.559823	3.919640	1.573889
55	1	0	2.100895	2.538839	-2.703911
56	1	0	2.645996	1.874629	1.110985
57	1	0	1.311592	7.644791	-0.141964
58	1	0	4.046522	1.599700	-0.858697
59	1	0	2.622657	5.075086	-2.396789
60	1	0	3.313366	4.217103	1.503904
61	1	0	2.918938	5.865382	-0.089753
62	1	0	4.721909	2.653330	0.403627
63	1	0	4.425504	3.370962	-2.369649
64	1	0	4.738387	4.522927	-1.058163
65	7	0	2.627524	2.620916	0.312961
66	6	0	1.068599	-0.871234	3.011581
67	6	0	-1.184199	-1.318328	2.020939
68	6	0	-1.390441	-2.300192	-0.359103
69	6	0	-1.961121	-1.724212	0.788496
70	6	0	-2.196560	-2.525868	-1.478653
71	6	0	-3.328494	-1.408123	0.788874
72	6	0	-3.551018	-2.196119	-1.513807
73	6	0	-4.089237	-1.633747	-0.355811
74	1	0	0.467581	-0.793240	3.923837
75	1	0	0.634327	-1.564074	1.062975
76	1	0	-0.341215	-2.567417	-0.420994
77	1	0	-3.781660	-0.967936	1.669652
78	1	0	-4.149047	-2.347111	-2.406253
79	7	0	0.161698	-1.319043	1.936493
80	7	0	-1.569055	-3.095393	-2.717322
81	7	0	-5.523044	-1.196162	-0.362254
82	8	0	-0.349750	-3.268311	-2.702677
83	8	0	-1.801125	-0.947565	3.043953
84	8	0	-2.306646	-3.333257	-3.667240
85	8	0	-5.957340	-0.671274	0.664038
86	8	0	-6.159928	-1.362575	-1.396662
87	6	0	1.545896	0.562316	2.600133
88	8	0	0.718035	1.515211	2.738489
89	8	0	2.680838	0.669522	2.055075
90	6	0	1.742650	-3.318566	3.512056
91	6	0	0.874749	-3.384227	4.781561
92	6	0	2.208455	-1.882255	3.198709
93	6	0	2.969690	-4.238397	3.639638
94	1	0	1.428378	-2.979320	5.643462
95	1	0	1.136620	-3.672776	2.662533
96	1	0	2.662014	-5.278521	3.815255
97	1	0	0.606607	-4.424246	5.012632
98	1	0	-0.058698	-2.814466	4.670716
99	1	0	3.598898	-3.923578	4.486314
100	1	0	2.845886	-1.515795	4.017745
101	1	0	2.825706	-1.876416	2.291291
102	1	0	3.585512	-4.208837	2.729210
103	11	0	-1.388253	1.251937	3.475539

$2_S Na^+$

E(RB97D) = -2718.74624108 A.U.
NImag = 0

Zero-point correction= 0.819094 (Hartree/Particle)
Thermal correction to Energy= 0.874057
Thermal correction to Enthalpy= 0.875001
Thermal correction to Gibbs Free Energy= 0.727928
Sum of electronic and zero-point Energies= -2717.927148
Sum of electronic and thermal Energies= -2717.872184
Sum of electronic and thermal Enthalpies= -2717.871240
Sum of electronic and thermal Free Energies= -2718.018313

E(RPBE1PBE) = -2717.37458519 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	1.254235	-0.630642	0.416184
4	6	0	-1.046343	-1.750504	0.330063
5	6	0	-1.088512	-1.731576	-1.091887
6	6	0	-1.240417	-1.751897	3.109249
7	6	0	1.894971	1.406447	1.516251
8	6	0	-2.084200	-2.442833	1.066610
9	6	0	1.840814	3.752414	3.553194
10	6	0	-2.101524	-2.413873	-1.767989
11	6	0	-3.083348	-3.159047	0.337508
12	6	0	2.993084	3.409182	2.590968
13	6	0	-3.091803	-3.147691	-1.036333
14	6	0	2.948887	4.296689	1.332418
15	6	0	4.347834	3.569549	3.301547
16	1	0	0.610488	-0.609020	3.102907
17	1	0	-0.365394	-1.141050	-1.646458
18	1	0	0.958673	0.054818	-0.381071
19	1	0	-1.358735	-1.716905	4.193047
20	1	0	0.869089	3.591268	3.074651
21	1	0	1.899066	3.135665	4.460515
22	1	0	1.918202	4.808034	3.844922
23	1	0	1.986788	4.196795	0.819875
24	1	0	3.692073	1.364779	2.425837
25	1	0	4.404348	2.924376	4.190592
26	1	0	-3.859841	-3.669020	0.903641
27	1	0	-3.868505	-3.659168	-1.600384
28	1	0	3.081887	5.344566	1.631956
29	1	0	3.750786	4.021622	0.635241
30	1	0	4.464847	4.609811	3.626781
31	1	0	5.177924	3.327152	2.621989

32	7	0	-2.149589	-2.456338	2.433748
33	7	0	2.907035	1.962497	2.201455
34	8	0	0.883862	1.959096	1.105225
35	8	0	2.133114	0.040322	1.332693
36	6	0	-1.309602	-1.720877	-3.928702
37	1	0	-0.287428	-2.085112	-3.749486
38	1	0	-1.377574	-0.647501	-3.717155
39	1	0	-1.614235	-1.931923	-4.956581
40	8	0	-2.250185	-2.453476	-3.100987
41	6	0	2.019841	-1.818396	-0.224285
42	6	0	2.632445	-2.822133	0.812139
43	6	0	3.703315	-5.004829	-1.114881
44	6	0	3.505229	-2.600775	-1.946271
45	6	0	4.124859	-3.033105	0.462352
46	6	0	4.448242	-6.103494	-1.288499
47	6	0	4.244831	-3.606214	-0.985269
48	6	0	4.235304	-0.740755	-0.592068
49	6	0	4.832322	-1.659932	0.518631
50	1	0	1.271822	-2.348567	-0.823073
51	1	0	2.136655	-3.809607	0.731271
52	1	0	2.612269	-5.104073	-1.084395
53	1	0	2.217907	-0.323914	-2.259927
54	1	0	2.541971	-2.442720	1.841167
55	1	0	2.626454	-3.075213	-2.406386
56	1	0	3.998804	-7.091263	-1.382563
57	1	0	4.170830	-2.273413	-2.753347
58	1	0	3.945565	0.240747	-0.218672
59	1	0	4.581439	-3.735735	1.169347
60	1	0	4.682423	-1.212737	1.510781
61	1	0	4.953814	-0.577741	-1.404262
62	1	0	5.535849	-6.041965	-1.352589
63	1	0	5.315091	-3.623120	-1.231841
64	1	0	5.911272	-1.796692	0.370911
65	7	0	3.041669	-1.384630	-1.221110
66	6	0	0.459822	2.424646	-2.509610
67	6	0	-1.748665	1.565373	-1.720769
68	6	0	-2.268589	1.516173	0.815664
69	6	0	-2.580915	1.174463	-0.509489
70	6	0	-3.037235	0.986063	1.857707
71	6	0	-3.690834	0.350380	-0.761519
72	6	0	-4.120418	0.136552	1.637980
73	6	0	-4.428104	-0.155090	0.308092
74	1	0	0.000837	2.158414	-3.467032
75	1	0	-0.159434	2.125522	-0.504724
76	1	0	-1.438415	2.163498	1.073509
77	1	0	-3.950994	0.095226	-1.784155
78	1	0	-4.686770	-0.289837	2.459102
79	7	0	-0.498985	2.041769	-1.460622
80	7	0	-2.637662	1.285114	3.271614
81	7	0	-5.554517	-1.104738	0.025120
82	8	0	-1.712148	2.076785	3.445020
83	8	0	-2.190727	1.392568	-2.858539
84	8	0	-3.239279	0.694719	4.166501
85	8	0	-5.853289	-1.291992	-1.151215
86	8	0	-6.079392	-1.657231	0.989622
87	6	0	1.701429	1.537728	-2.283670
88	8	0	1.498198	0.265615	-2.693202
89	8	0	2.713414	1.906787	-1.716274
90	6	0	-0.422494	4.845965	-2.652295
91	6	0	-1.061294	4.658095	-4.040281
92	6	0	0.007576	6.308669	-2.440503
93	6	0	0.793644	3.921720	-2.445883
94	1	0	-0.319884	4.857132	-4.830183
95	1	0	-0.850284	6.987038	-2.546062
96	1	0	-1.175438	4.595263	-1.887424
97	1	0	-1.455495	3.642420	-4.175253
98	1	0	-1.894288	5.361605	-4.176516
99	1	0	0.444613	6.455386	-1.441640
100	1	0	0.762011	6.597706	-3.188320
101	1	0	1.269783	4.129801	-1.477242
102	1	0	1.549332	4.133318	-3.218144
103	11	0	0.150506	-3.772272	1.885141

$3_S Na^+$

E(RB97D) = -2718.77215640 A.U.
NImag = 0

Zero-point correction= 0.819248 (Hartree/Particle)
Thermal correction to Energy= 0.874220
Thermal correction to Enthalpy= 0.875164
Thermal correction to Gibbs Free Energy= 0.727669
Sum of electronic and zero-point Energies= -2717.952909
Sum of electronic and thermal Energies= -2717.897937
Sum of electronic and thermal Enthalpies= -2717.896993
Sum of electronic and thermal Free Energies= -2718.044487

E(RPBE1PBE) = -2717.41251280 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.456634	-0.731091	-2.881639
2	6	0	-0.810292	-0.896086	-1.556068
3	6	0	-0.406269	-2.099174	-0.888601
4	6	0	-0.656086	-2.355959	0.492754
5	6	0	0.288059	-1.741635	-3.546340
6	6	0	1.409244	4.279520	-2.548384
7	6	0	-1.626085	0.144426	-0.806265
8	6	0	-0.213153	-3.543194	1.058372
9	6	0	0.320336	-3.067092	-1.671088
10	6	0	-0.563955	2.241077	-1.273699
11	6	0	0.501645	4.958772	-0.275583
12	6	0	0.470963	-4.521206	0.279475
13	6	0	0.728405	-4.285361	-1.055792
14	6	0	0.146565	4.620793	-1.736618
15	6	0	-0.597835	5.800902	-2.384248
16	1	0	-1.146755	-1.611857	1.114160
17	1	0	1.923223	3.417548	-2.112493
18	1	0	-0.735157	0.174347	-3.415317
19	1	0	0.576842	-1.600086	-4.589701
20	1	0	-1.183392	0.290230	0.179671
21	1	0	1.036024	4.127206	0.195309
22	1	0	2.096786	5.134790	-2.532290
23	1	0	1.147530	4.058523	-3.592199
24	1	0	1.147173	5.846666	-0.259156
25	1	0	-0.407088	5.166618	0.304091
26	1	0	0.748950	-5.467258	0.746319
27	1	0	1.257441	-5.012999	-1.665722
28	1	0	-1.722871	3.623288	-2.172108
29	1	0	0.055257	6.681341	-2.392422
30	1	0	-0.872846	5.567736	-3.423282
31	1	0	-1.505503	6.051799	-1.816002
32	7	0	0.663554	-2.876789	-2.979425
33	7	0	-0.805462	3.465365	-1.775607
34	8	0	0.465835	1.854089	-0.731476
35	8	0	-1.666974	1.416838	-1.478822
36	6	0	-1.151259	-3.018693	3.229809
37	1	0	-2.180282	-3.051795	2.848211
38	1	0	-0.796745	-1.982543	3.234449
39	1	0	-1.102252	-3.460180	4.229222
40	8	0	-0.300768	-3.855767	2.398534
41	6	0	-3.071425	-0.367813	-0.627463
42	6	0	-3.961567	-0.327433	-1.900279
43	6	0	-5.020917	-0.472324	0.855283
44	6	0	-6.337492	-1.936074	-0.751319
45	6	0	-4.199403	1.747397	0.190501
46	6	0	-5.996191	-0.518689	-0.369565
47	6	0	-7.583168	-2.418092	-0.826376
48	6	0	-5.332293	0.282317	-1.531430
49	6	0	-5.109432	1.740021	-1.068049
50	1	0	-2.974939	-1.399897	-0.274589
51	1	0	-3.112519	0.310361	1.397862
52	1	0	-4.077121	-1.340210	-2.301198
53	1	0	-4.677646	-1.472277	1.146932
54	1	0	-5.491404	-2.591832	-0.976893
55	1	0	-3.491195	0.288729	-2.674559
56	1	0	-3.282199	2.322296	0.077156
57	1	0	-7.779437	-3.449455	-1.116142
58	1	0	-5.477305	0.005071	1.728670
59	1	0	-4.716675	2.114815	1.083149
60	1	0	-5.995473	0.258134	-2.403427
61	1	0	-4.635260	2.309405	-1.877514
62	1	0	-6.924122	0.003313	-0.099441
63	1	0	-8.445778	-1.789081	-0.599487
64	1	0	-6.073332	2.213313	-0.842424
65	7	0	-3.791986	0.329745	0.515257
66	6	0	0.100628	0.964488	3.044845
67	6	0	1.750271	-0.375408	1.723233
68	6	0	3.155517	0.750195	-0.084821
69	6	0	2.584540	-0.407149	0.467304
70	6	0	3.943838	0.639216	-1.231723
71	6	0	2.840477	-1.645195	-0.131154
72	6	0	4.213426	-0.584420	-1.847915
73	6	0	3.661106	-1.719753	-1.255041
74	1	0	0.879440	1.345964	1.094430
75	1	0	0.125012	0.072222	3.674403
76	1	0	2.995289	1.726872	0.358995
77	1	0	2.365577	-2.551756	0.222928
78	1	0	4.833484	-0.649927	-2.736723
79	7	0	0.985750	0.710367	1.890281
80	7	0	4.524553	1.890568	-1.830782
81	7	0	3.983699	-3.069491	-1.811256
82	8	0	4.435591	2.921685	-1.169045
83	8	0	1.813377	-1.326432	2.538623
84	8	0	5.032180	1.793486	-2.943245
85	8	0	3.779797	-4.035892	-1.067027
86	8	0	4.440535	-3.127810	-2.942813
87	6	0	-1.317634	1.143183	2.419508
88	8	0	-2.077845	0.099332	2.460766
89	8	0	-1.568492	2.208707	1.832520
90	6	0	2.396737	3.435708	5.042517
91	6	0	0.571771	2.204176	3.821318
92	6	0	1.997800	2.096635	4.397244
93	6	0	2.123480	0.944078	5.411036

94	1	0	2.334220	4.259990	4.317450
95	1	0	1.725588	3.670362	5.882840
96	1	0	1.414098	1.090887	6.240446
97	1	0	0.490323	3.074248	3.155043
98	1	0	3.423920	3.393499	5.431111
99	1	0	-0.140574	2.368317	4.645391
100	1	0	2.690608	1.900173	3.561795
101	1	0	1.918614	-0.030035	4.946046
102	1	0	3.136685	0.912351	5.836093
103	11	0	2.192437	-3.529078	2.352281

$1_R Na^+$

E(RB97D) = -2718.79542446 A.U.
NImag = 0

Zero-point correction= 0.819631 (Hartree/Particle)
Thermal correction to Energy= 0.874593
Thermal correction to Enthalpy= 0.875537
Thermal correction to Gibbs Free Energy= 0.729038
Sum of electronic and zero-point Energies= -2717.975794
Sum of electronic and thermal Energies= -2717.920831
Sum of electronic and thermal Enthalpies= -2717.919887
Sum of electronic and thermal Free Energies= -2718.066386

E(RPBE1PBE) = -2717.43650235 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.280058	0.461426	-1.731259
2	6	0	0.373589	-0.135990	-2.974928
3	6	0	1.457234	0.438482	-0.762998
4	6	0	-0.712840	-0.056319	-3.885699
5	6	0	-0.936824	1.145654	-1.395991
6	6	0	-1.199762	1.750054	-0.137142
7	6	0	2.432539	-1.777238	-0.758188
8	6	0	2.537500	-4.799593	-1.484135
9	6	0	-1.953665	1.202378	-2.419528
10	6	0	-2.401083	2.412824	0.086800
11	6	0	3.726398	-3.934304	-1.027875
12	6	0	-3.156263	1.910820	-2.154668
13	6	0	-3.383087	2.513161	-0.932701
14	6	0	4.976942	-4.273165	-1.857390
15	6	0	4.015803	-4.134768	0.471678
16	1	0	1.272264	-0.674089	-3.263202
17	1	0	1.111736	0.124298	0.224485
18	1	0	-0.477635	1.679139	0.673599
19	1	0	-0.638938	-0.550235	-4.856144
20	1	0	2.336422	-4.649718	-2.552721
21	1	0	1.633248	-4.551847	-0.919604
22	1	0	4.040772	-2.002750	-1.951680
23	1	0	2.780557	-5.857232	-1.316756
24	1	0	4.788031	-4.120698	-2.929965
25	1	0	3.140826	-3.869312	1.074983
26	1	0	-3.904527	1.950478	-2.943276
27	1	0	5.238661	-5.326390	-1.703235
28	1	0	5.833463	-3.656785	-1.547314
29	1	0	-4.320095	3.032140	-0.759151
30	1	0	4.260581	-5.189620	0.652428
31	1	0	4.869134	-3.518339	0.785982
32	7	0	-1.834735	0.597811	-3.638101
33	7	0	3.439988	-2.486832	-1.296760
34	8	0	2.495647	-0.457575	-1.201412
35	8	0	1.578590	-2.191601	0.017389
36	6	0	-3.818045	3.649108	1.624889
37	1	0	-3.744098	3.989152	2.663107
38	1	0	-3.918706	4.517516	0.960222
39	1	0	-4.678594	2.976848	1.504374
40	8	0	-2.580593	2.946901	1.352183
41	6	0	2.054071	1.853479	-0.643339
42	6	0	2.579816	2.492100	-1.946709
43	6	0	3.161701	3.400357	0.887704
44	6	0	2.073346	5.168707	-0.604229
45	6	0	3.315983	4.351455	-0.349321
46	6	0	4.517037	1.596373	-0.098132
47	6	0	3.721301	3.468703	-1.574062
48	6	0	2.056726	6.504245	-0.681166
49	6	0	4.953634	2.626435	-1.174826
50	1	0	1.242807	2.469557	-0.249878
51	1	0	2.229533	3.558602	1.439821
52	1	0	2.916434	1.311420	1.268120
53	1	0	1.753778	3.005765	-2.449664
54	1	0	1.140918	4.613560	-0.740322
55	1	0	2.959803	1.721014	-2.629106
56	1	0	4.002567	3.493269	1.583571
57	1	0	4.443826	0.582105	-0.489967
58	1	0	1.137193	7.052784	-0.880804
59	1	0	5.173592	1.591006	0.778254
60	1	0	3.958796	4.119575	-2.422254
61	1	0	5.349651	2.099596	-2.051683
62	1	0	4.148363	5.039164	-0.149586
63	1	0	2.968873	7.088680	-0.548574
64	1	0	5.746960	3.279262	-0.788308
65	7	0	3.142152	1.965459	0.417840
66	6	0	-1.557329	-0.948099	1.850900
67	6	0	0.670584	-0.935590	3.096053
68	6	0	-1.641816	-2.090377	-0.476396
69	6	0	-2.226577	-1.314548	0.538927
70	6	0	-2.327552	-2.264202	-1.682261
71	6	0	-3.492225	-0.747914	0.319169
72	6	0	-3.571781	-1.688139	-1.935295
73	6	0	-4.130731	-0.931548	-0.904572
74	1	0	-0.665993	-2.553969	-0.378998
75	1	0	0.224693	-1.731199	1.220457
76	1	0	1.427150	-1.725424	3.085546
77	1	0	-3.959841	-0.151019	1.093454
78	1	0	-4.068427	-1.803602	-2.892835
79	7	0	-0.268085	-1.313059	2.010215
80	7	0	-1.674419	-3.063568	-2.771329
81	7	0	-5.438192	-0.237020	-1.141819
82	8	0	-0.553981	-3.520113	-2.540662
83	8	0	-2.211783	-0.311319	2.702061
84	8	0	-2.289886	-3.196580	-3.823371
85	8	0	-5.894320	0.438471	-0.218314
86	8	0	-5.953239	-0.364626	-2.247287
87	6	0	1.397193	0.376476	2.658458
88	8	0	0.732326	1.453722	2.594920
89	8	0	2.607564	0.252760	2.309575
90	6	0	0.077526	-0.858897	4.509577
91	6	0	-1.253117	-1.895494	6.373244
92	6	0	-0.682255	-2.122590	4.962762
93	6	0	0.218944	-3.370399	4.932333
94	1	0	-0.584753	0.010733	4.609113
95	1	0	-1.920164	-1.020696	6.394823
96	1	0	-1.523203	-2.276077	4.272330
97	1	0	-1.827134	-2.770302	6.707636
98	1	0	0.928922	-0.690303	5.188019
99	1	0	-0.440284	-1.726179	7.096156
100	1	0	0.568003	-3.599683	3.915676
101	1	0	-0.328569	-4.247034	5.304060
102	1	0	1.100605	-3.223613	5.575392
103	11	0	-1.423143	1.752929	3.127668

$2_R Na^+$

E(RB97D) = -2718.76130063 A.U.
NImag = 0

Zero-point correction= 0.818339 (Hartree/Particle)
Thermal correction to Energy= 0.873893
Thermal correction to Enthalpy= 0.874837
Thermal correction to Gibbs Free Energy= 0.724517
Sum of electronic and zero-point Energies= -2717.942962
Sum of electronic and thermal Energies= -2717.887408
Sum of electronic and thermal Enthalpies= -2717.886464
Sum of electronic and thermal Free Energies= -2718.036784

E(RPBE1PBE) = -2717.40314546 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.020754	0.025334	-1.828143
2	6	0	0.285865	0.930747	-2.826916
3	6	0	0.698397	-2.045412	-0.588287
4	6	0	0.917782	-1.019975	-1.553004
5	6	0	-0.973416	5.053945	1.113079
6	6	0	-1.312912	0.090680	-1.039309
7	6	0	1.523627	0.825475	-3.514900
8	6	0	-1.699996	2.232457	0.021315
9	6	0	1.677631	-2.989156	-0.352167
10	6	0	2.156835	-1.012660	-2.288323
11	6	0	-2.394474	4.534019	0.826887
12	6	0	2.910958	-2.976301	-1.048149
13	6	0	-3.079458	4.079700	2.128870
14	6	0	3.141478	-2.001335	-2.000881
15	6	0	-3.228358	5.633211	0.146063
16	1	0	-0.233518	-2.103457	-0.032010
17	1	0	-0.399586	1.739051	-3.065023
18	1	0	-0.365146	4.275975	1.586845
19	1	0	-0.484392	5.374773	0.185902
20	1	0	-1.108380	-0.159281	0.004662
21	1	0	-1.041519	5.911401	1.795726
22	1	0	1.764068	1.545755	-4.299361
23	1	0	-2.504347	3.281861	2.609491
24	1	0	-2.811561	3.525058	-1.038451
25	1	0	-2.752539	5.960794	-0.789339
26	1	0	-3.144363	4.932640	2.817347
27	1	0	-3.302053	6.498418	0.815173
28	1	0	3.662659	-3.731898	-0.826040
29	1	0	4.075894	-1.966487	-2.556597

30	1	0	-4.095179	3.715991	1.923508
31	1	0	-4.246333	5.277460	-0.069937
32	7	0	-2.354466	3.394421	-0.144603
33	7	0	2.445788	-0.087835	-3.252812
34	8	0	-1.053653	1.903695	1.021636
35	8	0	-1.876757	1.424089	-1.079907
36	6	0	0.955946	-5.225653	0.053729
37	1	0	-0.011662	-5.051098	-0.437618
38	1	0	0.833160	-5.925444	0.888385
39	1	0	1.678591	-5.625242	-0.671279
40	8	0	1.450623	-3.979619	0.620055
41	6	0	-2.334960	-0.945659	-1.551615
42	6	0	-3.022292	-0.586485	-2.906065
43	6	0	-3.967724	-3.469982	-3.299733
44	6	0	-3.944002	-2.584397	-0.897973
45	6	0	-4.620554	-4.424139	-3.975522
46	6	0	-4.402410	-0.280759	-0.397815
47	6	0	-4.502962	-1.024762	-2.803398
48	6	0	-4.606165	-2.509563	-2.334241
49	6	0	-5.189610	-0.134495	-1.744225
50	1	0	-1.745299	-1.860166	-1.701892
51	1	0	-2.512809	-1.090871	-3.736028
52	1	0	-2.887359	-3.362641	-3.440819
53	1	0	-2.983722	0.493747	-3.096039
54	1	0	-3.165924	-3.361848	-0.877522
55	1	0	-4.105446	-5.092552	-4.664861
56	1	0	-3.954375	0.670978	-0.102744
57	1	0	-4.698627	-2.843138	-0.143497
58	1	0	-4.995749	-0.917753	-3.777133
59	1	0	-5.065941	-0.598977	0.416293
60	1	0	-5.186224	0.911766	-2.080956
61	1	0	-5.697557	-4.558871	-3.859166
62	1	0	-5.673896	-2.757532	-2.250487
63	1	0	-6.236923	-0.442825	-1.619919
64	7	0	-3.322389	-1.299573	-0.496721
65	6	0	-0.038018	-1.204012	2.803079
66	6	0	1.968523	-0.344538	1.773951
67	6	0	2.055966	1.644389	0.157725
68	6	0	2.666345	0.550526	0.792396
69	6	0	2.764880	2.334262	-0.827263
70	6	0	3.971876	0.179802	0.427367
71	6	0	4.059326	1.984792	-1.213823
72	6	0	4.637944	0.897492	-0.562641
73	1	0	0.099140	0.609709	1.655096
74	1	0	0.130387	-2.152626	2.269459
75	1	0	1.045173	1.960847	0.392157
76	1	0	4.448699	-0.675212	0.892733
77	1	0	4.583519	2.519627	-1.999028
78	7	0	0.656014	-0.155719	2.053958
79	7	0	2.084152	3.454638	-1.552354
80	7	0	6.008907	0.450074	-0.984574
81	8	0	0.920344	3.704735	-1.236432
82	8	0	2.593282	-1.300291	2.284893
83	8	0	2.718079	4.032627	-2.428303
84	8	0	6.397190	-0.636656	-0.558160
85	8	0	6.636402	1.191454	-1.731503
86	6	0	0.584191	-1.424781	4.189315
87	1	0	1.250264	-0.519149	5.705771
88	8	0	0.871194	-0.289030	4.837997
89	8	0	0.785424	-2.541956	4.652670
90	6	0	-1.574915	-1.012263	2.842264
91	6	0	-2.144094	0.162885	3.674430
92	6	0	-2.375809	-0.232999	5.146391
93	6	0	-3.480838	0.612392	3.057344
94	1	0	-1.438982	1.005471	3.629486
95	1	0	-1.469961	-0.598520	5.643357
96	1	0	-1.901952	-0.933864	1.794597
97	1	0	-1.996941	-1.957320	3.215507
98	1	0	-2.746308	0.628262	5.718839
99	1	0	-3.136106	-1.026902	5.201306
100	1	0	-3.338866	0.965359	2.030836
101	1	0	-3.926630	1.423348	3.647970
102	1	0	-4.191527	-0.227661	3.040854
103	11	0	2.130907	-3.453462	2.839252

$3_R Na^+$

E(RB97D) = -2718.77730562 A.U.
NImag = 0

Zero-point correction= 0.818882 (Hartree/Particle)
Thermal correction to Energy= 0.874210
Thermal correction to Enthalpy= 0.875154
Thermal correction to Gibbs Free Energy= 0.724709
Sum of electronic and zero-point Energies= -2717.958424
Sum of electronic and thermal Energies= -2717.903095
Sum of electronic and thermal Enthalpies= -2717.902151
Sum of electronic and thermal Free Energies= -2718.052597

E(RPBE1PBE) = -2717.42381111 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.168691	-1.747269	-1.489087
2	6	0	0.747396	1.870107	-4.175913
3	6	0	0.985204	0.770664	-3.307366
4	6	0	1.162423	3.387522	-2.503836
5	6	0	1.265316	4.747725	-2.102292
6	6	0	1.315217	0.994463	-1.983575
7	6	0	1.409058	2.351943	-1.529258
8	6	0	1.592597	-0.159710	-1.028998
9	6	0	-1.718268	-4.326670	-3.700492
10	6	0	1.593942	5.092914	-0.805162
11	6	0	-1.841667	-3.314587	-2.549136
12	6	0	1.742018	2.727949	-0.199996
13	6	0	1.827480	4.069230	0.150055
14	6	0	-2.259656	-4.037342	-1.255870
15	6	0	-2.854406	-2.213668	-2.922156
16	1	0	0.246308	-2.994821	-3.024063
17	1	0	0.481527	1.683003	-5.218446
18	1	0	-0.990032	-5.113383	-3.455389
19	1	0	0.899086	-0.241904	-3.692438
20	1	0	1.040542	0.013134	-0.095237
21	1	0	1.074131	5.512048	-2.852397
22	1	0	-1.411666	-3.826542	-4.630832
23	1	0	-1.551288	-4.843557	-1.023703
24	1	0	1.661947	6.140516	-0.526290
25	1	0	1.928494	1.966507	0.554229
26	1	0	-2.291451	-3.337126	-0.415378
27	1	0	-2.559577	-1.725446	-3.861092
28	1	0	-2.691493	-4.801089	-3.871918
29	1	0	-2.912109	-1.458123	-2.131777
30	1	0	-3.260912	-4.466036	-1.383786
31	1	0	-3.845669	-2.664767	-3.057241
32	7	0	-0.479912	-2.714283	-2.377450
33	7	0	0.833382	3.135456	-3.806022
34	8	0	-0.909780	-1.226939	-0.671376
35	8	0	1.188399	-1.423855	-1.599504
36	6	0	2.464807	5.688916	1.854797
37	1	0	1.601325	6.358755	1.737881
38	1	0	2.763057	5.638244	2.906375
39	1	0	3.304478	6.044868	1.242967
40	8	0	2.116818	4.334426	1.481876
41	6	0	3.088091	-2.441690	0.520695
42	6	0	3.102359	-0.236652	-0.717301
43	6	0	3.937762	-3.061153	-0.622373
44	6	0	3.998693	-0.857523	-1.826168
45	6	0	4.801209	-0.738997	0.991100
46	6	0	4.868349	-1.973432	-1.205353
47	6	0	5.754690	-1.403354	-0.054911
48	6	0	6.800565	-0.432638	-0.539874
49	6	0	8.118774	-0.647448	-0.465811
50	1	0	2.017476	-2.572505	0.365142
51	1	0	2.736923	-0.493521	1.374020
52	1	0	3.277867	-3.441598	-1.410961
53	1	0	3.351497	-2.842811	1.505731
54	1	0	3.377579	-1.280992	-2.621880
55	1	0	3.423361	0.788303	-0.510758
56	1	0	4.531525	-3.899628	-0.238214
57	1	0	4.625517	-0.078012	-2.271895
58	1	0	4.922245	-1.159739	1.994658
59	1	0	4.943776	0.345859	1.053347
60	1	0	5.518193	-2.406915	-1.973571
61	1	0	6.263244	-2.253454	0.420350
62	1	0	6.428675	0.498292	-0.976929
63	1	0	8.517614	-1.563814	-0.027158
64	1	0	8.836964	0.080824	-0.839711
65	7	0	3.360431	-0.959574	0.596216
66	6	0	0.142771	-1.111319	2.532514
67	6	0	-1.536340	0.481154	1.599361
68	6	0	-2.949950	0.599232	1.090433
69	6	0	-3.495730	1.882627	0.934582
70	6	0	-3.681274	-0.521251	0.669298
71	6	0	-4.768364	2.019470	0.380420
72	6	0	-4.945837	-0.337808	0.105444
73	6	0	-5.519576	0.924564	-0.052543
74	1	0	0.567202	-1.426407	1.570073
75	1	0	-1.967889	-1.325004	2.426683
76	1	0	-2.928642	2.760955	1.225668
77	1	0	-3.264217	-1.521490	0.715186
78	1	0	-6.500031	1.050981	-0.501048
79	7	0	-1.228003	-0.654285	2.267670
80	7	0	-5.345669	3.401391	0.219433
81	7	0	-5.698667	-1.542427	-0.382018
82	8	0	-0.724981	1.398496	1.382712
83	8	0	-4.650402	4.344211	0.591297
84	8	0	-5.215970	-2.645979	-0.126745
85	8	0	-6.465011	3.487706	-0.273009
86	8	0	-6.734863	-1.346280	-1.006938
87	6	0	1.003207	0.053364	3.093213
88	8	0	0.580518	0.694934	4.068950
89	8	0	2.094877	0.330414	2.451846
90	6	0	0.134442	-2.292061	3.518742
91	6	0	-0.027714	-4.112401	1.729706

92	6	0	-0.567781	-4.625028	4.150283
93	6	0	-0.611258	-3.558808	3.040985
94	1	0	-0.285690	-1.936901	4.469903
95	1	0	-0.118603	-3.391951	0.906549
96	1	0	0.473984	-4.912904	4.359119
97	1	0	-0.553263	-5.029050	1.431608
98	1	0	-1.009726	-4.246811	5.082312
99	1	0	1.035734	-4.361968	1.868194
100	1	0	-1.116267	-5.527087	3.846849
101	1	0	1.183788	-2.563407	3.715390
102	1	0	-1.674030	-3.315243	2.865749
103	11	0	0.919233	2.621317	2.637411

$1_S Li^+$

E(RB97D) = -2564.07963844 A.U.
NImag = 0

Zero-point correction= 0.820565 (Hartree/Particle)
Thermal correction to Energy= 0.875058
Thermal correction to Enthalpy= 0.876002
Thermal correction to Gibbs Free Energy= 0.729957
Sum of electronic and zero-point Energies= -2563.259074
Sum of electronic and thermal Energies= -2563.204581
Sum of electronic and thermal Enthalpies= -2563.203637
Sum of electronic and thermal Free Energies= -2563.349682

E(RPBE1PBE) = -2562.76978024 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.074532	0.830950	-1.498869
2	6	0	-0.176472	0.409156	-2.811237
3	6	0	1.234471	0.710131	-0.727073
4	6	0	2.274261	-4.412919	-2.122910
5	6	0	-1.282370	1.850859	0.464628
6	6	0	-1.232017	1.413440	-0.882795
7	6	0	2.213132	-1.478438	-1.085801
8	6	0	-1.405375	0.556396	-3.509439
9	6	0	-2.450915	2.386181	0.990695
10	6	0	3.494384	-3.565008	-1.719650
11	6	0	-2.418271	1.535254	-1.695010
12	6	0	4.647434	-3.787681	-2.713259
13	6	0	-3.611743	2.539399	0.190927
14	6	0	3.954640	-3.905455	-0.289316
15	6	0	-3.583204	2.117582	-1.125580
16	1	0	0.670795	-0.050342	-3.312298
17	1	0	-0.415004	1.756947	1.113545
18	1	0	1.946543	-4.164421	-3.140409
19	1	0	1.038554	0.282770	0.259965
20	1	0	1.439584	-4.247576	-1.434269
21	1	0	2.551697	-5.474864	-2.092205
22	1	0	3.642877	-1.553181	-2.503748
23	1	0	-1.482838	0.203310	-4.539321
24	1	0	4.336138	-3.534657	-3.737276
25	1	0	3.146291	-3.734282	0.429267
26	1	0	4.939609	-4.844054	-2.697427
27	1	0	4.243139	-4.963834	-0.247791
28	1	0	5.524869	-3.183589	-2.440134
29	1	0	-4.524221	2.960030	0.601650
30	1	0	4.823185	-3.294990	-0.006667
31	1	0	-4.463969	2.208573	-1.757906
32	7	0	3.159234	-2.105178	-1.806733
33	7	0	-2.491512	1.101572	-2.987969
34	8	0	1.482382	-1.986870	-0.242312
35	8	0	2.187100	-0.125217	-1.414091
36	6	0	-3.601187	3.243000	2.959283
37	1	0	-3.905168	4.181053	2.477198
38	1	0	-3.330428	3.431269	4.002249
39	1	0	-4.409729	2.501981	2.900076
40	8	0	-2.398892	2.729559	2.330707
41	6	0	1.856941	2.107210	-0.540321
42	6	0	2.295390	2.834801	-1.830672
43	6	0	3.140800	3.520662	0.993851
44	6	0	4.342606	1.726944	-0.194453
45	6	0	3.519427	3.718107	-1.495314
46	6	0	2.061192	5.441832	-0.293765
47	6	0	4.731185	2.788753	-1.259634
48	6	0	3.265819	4.539328	-0.190469
49	6	0	2.120928	6.778027	-0.284429
50	1	0	1.090436	2.703068	-0.038131
51	1	0	1.457911	3.432356	-2.205768
52	1	0	2.836399	1.427955	1.261985
53	1	0	2.565768	2.108672	-2.607032
54	1	0	2.251805	3.689329	1.610736
55	1	0	4.205909	0.732855	-0.619941
56	1	0	1.089113	4.949211	-0.385683
57	1	0	5.009140	2.289515	-2.196039
58	1	0	4.023747	3.531096	1.641760
59	1	0	5.062216	1.664504	0.628479
60	1	0	3.723749	4.411032	-2.318504
61	1	0	1.224095	7.389627	-0.372561
62	1	0	4.153507	5.160935	-0.014754
63	1	0	5.595545	3.375541	-0.922905
64	1	0	3.074683	7.299919	-0.188747
65	7	0	3.024402	2.118398	0.441816
66	6	0	0.763810	-1.045388	3.107335
67	6	0	-1.457774	-0.962320	1.980027
68	6	0	-1.770030	-1.872731	-0.410699
69	6	0	-2.278492	-1.264450	0.750717
70	6	0	-2.597639	-2.002560	-1.527768
71	6	0	-3.606501	-0.810482	0.760020
72	6	0	-3.917421	-1.550525	-1.548663
73	6	0	-4.392671	-0.954565	-0.381066
74	1	0	0.149676	-0.906294	4.003281
75	1	0	0.287050	-1.698655	1.152005
76	1	0	-0.748179	-2.226787	-0.492508
77	1	0	-4.010366	-0.329786	1.643517
78	1	0	-4.533778	-1.633624	-2.437628
79	7	0	-0.161720	-1.321675	1.988809
80	7	0	-2.025745	-2.596465	-2.781024
81	7	0	-5.781641	-0.385006	-0.373947
82	8	0	-0.820580	-2.853564	-2.783536
83	8	0	-1.990520	-0.355397	2.942185
84	8	0	-2.787625	-2.767254	-3.725643
85	8	0	-6.146778	0.193621	0.649250
86	8	0	-6.447962	-0.512985	-1.395012
87	6	0	1.452470	0.314111	2.763192
88	8	0	0.753363	1.368122	2.908879
89	8	0	2.608509	0.282010	2.263513
90	6	0	0.121149	-3.562349	4.744778
91	6	0	1.055963	-3.583167	3.521897
92	6	0	1.735388	-2.218410	3.284474
93	6	0	2.136334	-4.668358	3.674862
94	1	0	-0.714201	-2.860150	4.611759
95	1	0	-0.304824	-4.559194	4.922575
96	1	0	0.452722	-3.824262	2.631545
97	1	0	0.678544	-3.267219	5.647512
98	1	0	2.381023	-2.269129	2.398502
99	1	0	2.386911	-1.979393	4.138198
100	1	0	1.680209	-5.660633	3.794859
101	1	0	2.754998	-4.468931	4.563033
102	1	0	2.798902	-4.695080	2.797603
103	3	0	-1.111464	1.323921	3.183069

$1_R Li^+$

E(RB97D) = -2564.07519824 A.U.
NImag = 0

Zero-point correction= 0.821183 (Hartree/Particle)
Thermal correction to Energy= 0.875472
Thermal correction to Enthalpy= 0.876416
Thermal correction to Gibbs Free Energy= 0.731758
Sum of electronic and zero-point Energies= -2563.254015
Sum of electronic and thermal Energies= -2563.199727
Sum of electronic and thermal Enthalpies= -2563.198782
Sum of electronic and thermal Free Energies= -2563.343440

E(RPBE1PBE) = -2562.76590500 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368237	-0.546409	-1.640219
2	6	0	-0.350377	0.003886	-2.908232
3	6	0	-1.533388	-0.307376	-0.686523
4	6	0	0.733656	-1.376504	-1.247643
5	6	0	0.870128	-1.959737	0.037050
6	6	0	0.739623	-0.262671	-3.780690
7	6	0	-2.142318	2.035640	-0.724195
8	6	0	-1.791214	5.028738	-1.497499
9	6	0	1.770266	-1.601705	-2.224884
10	6	0	1.976726	-2.738794	0.345873
11	6	0	-3.093632	4.362335	-1.018695
12	6	0	2.869071	-2.434432	-1.878549
13	6	0	2.982026	-2.997418	-0.620508
14	6	0	-4.287088	4.875502	-1.842436
15	6	0	-3.332891	4.625477	0.479984
16	1	0	-1.156253	0.651345	-3.242659
17	1	0	-1.143908	-0.024117	0.295066
18	1	0	0.126264	-1.781964	0.809680
19	1	0	-1.624872	4.834745	-2.564846
20	1	0	-0.931136	4.652976	-0.934334
21	1	0	0.754871	0.190270	-4.773623
22	1	0	-1.867000	6.113491	-1.345384
23	1	0	-3.695459	2.490969	-1.924092
24	1	0	-4.135273	4.682954	-2.914481
25	1	0	-2.499571	4.242218	1.078788
26	1	0	-4.385832	5.957953	-1.700965
27	1	0	-5.223725	4.399790	-1.516544

28	1	0	3.634005	-2.603164	-2.633775
29	1	0	3.846279	-3.608904	-0.380762
30	1	0	-3.417185	5.707389	0.645859
31	1	0	-4.264216	4.146508	0.811745
32	7	0	-3.034272	2.883747	-1.266108
33	7	0	1.763350	-1.040297	-3.469900
34	8	0	-2.406252	0.736581	-1.157838
35	8	0	-1.236657	2.318722	0.051433
36	6	0	3.198528	-3.966915	2.055637
37	1	0	3.033883	-4.217468	3.107688
38	1	0	3.279222	-4.886240	1.461428
39	1	0	4.105394	-3.357506	1.943126
40	8	0	2.029587	-3.212354	1.645918
41	6	0	-2.355507	-1.601407	-0.531988
42	6	0	-3.050077	-2.126447	-1.808595
43	6	0	-3.674989	-2.938976	1.040958
44	6	0	-4.689186	-0.874168	0.153753
45	6	0	-3.083095	-4.872120	-0.513820
46	6	0	-4.358389	-2.835565	-1.387501
47	6	0	-4.101396	-3.806226	-0.191234
48	6	0	-5.364725	-1.754807	-0.932687
49	6	0	-3.368437	-6.173770	-0.629057
50	1	0	-1.649470	-2.356207	-0.176891
51	1	0	-3.000092	-0.959116	1.427794
52	1	0	-2.760374	-3.302012	1.521661
53	1	0	-2.370259	-2.810655	-2.327348
54	1	0	-3.281699	-1.298969	-2.490689
55	1	0	-2.054139	-4.533063	-0.664594
56	1	0	-4.435099	0.122243	-0.207307
57	1	0	-4.465658	-2.874682	1.796098
58	1	0	-5.291979	-0.779723	1.062961
59	1	0	-2.601161	-6.906171	-0.875950
60	1	0	-5.657210	-1.130983	-1.786234
61	1	0	-4.766075	-3.407132	-2.228118
62	1	0	-5.055611	-4.294912	0.045404
63	1	0	-6.272222	-2.228401	-0.536558
64	1	0	-4.383958	-6.544544	-0.479451
65	7	0	-3.391852	-1.525697	0.586434
66	6	0	-0.367753	0.998565	3.143726
67	6	0	1.733222	0.600372	1.775751
68	6	0	1.943723	1.722450	-0.542710
69	6	0	2.452075	0.900776	0.478988
70	6	0	2.640621	1.819004	-1.749059
71	6	0	3.657610	0.213691	0.264685
72	6	0	3.828443	1.130296	-1.994584
73	6	0	4.315050	0.335518	-0.957250
74	1	0	1.013423	2.272867	-0.453359
75	1	0	0.133821	1.765904	1.260214
76	1	0	-1.016816	1.878280	3.135395
77	1	0	4.061806	-0.430465	1.036840
78	1	0	4.334675	1.191561	-2.952204
79	7	0	0.562694	1.222930	2.008067
80	7	0	2.055903	2.654037	-2.850096
81	7	0	5.553910	-0.479776	-1.189706
82	8	0	0.968583	3.190816	-2.632881
83	8	0	2.237029	-0.230939	2.567124
84	8	0	2.688031	2.733288	-3.897220
85	8	0	5.932248	-1.203374	-0.268484
86	8	0	6.089228	-0.389851	-2.288959
87	6	0	-1.267642	-0.223560	2.788191
88	8	0	-0.731195	-1.375794	2.736032
89	8	0	-2.467846	0.024473	2.491449
90	6	0	0.292985	0.884123	4.526091
91	6	0	1.859779	1.791258	6.269445
92	6	0	1.264330	2.031062	4.871147
93	6	0	0.580191	3.407852	4.796368
94	1	0	0.817378	-0.074439	4.623050
95	1	0	2.369284	0.818015	6.321786
96	1	0	2.086994	2.007957	4.141069
97	1	0	2.588153	2.573875	6.522004
98	1	0	-0.531100	0.876724	5.257093
99	1	0	1.067374	1.805616	7.033377
100	1	0	0.224502	3.636764	3.781680
101	1	0	1.281319	4.200392	5.091025
102	1	0	-0.281805	3.447384	5.480385
103	3	0	1.101350	-1.733243	2.800334

$1_S K^+$

E(RB97D) =-3156.53515002 A.U.
NImag = 0

Zero-point correction= 0.819906 (Hartree/Particle)
Thermal correction to Energy= 0.875170
Thermal correction to Enthalpy= 0.876115
Thermal correction to Gibbs Free Energy= 0.728215
Sum of electronic and zero-point Energies= -3155.715244
Sum of electronic and thermal Energies= -3155.659980
Sum of electronic and thermal Enthalpies= -3155.659035
Sum of electronic and thermal Free Energies= -3155.806935

E(RPBE1PBE) = -3155.00873196 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.143106	0.053217	-1.994373
2	6	0	0.245779	0.988911	-3.009004
3	6	0	-1.114174	-0.072054	-1.145918
4	6	0	1.260588	-0.807622	-1.744041
5	6	0	1.263882	-1.841457	-0.766294
6	6	0	1.456572	1.101991	-3.740836
7	6	0	-2.068195	1.953094	-0.199520
8	6	0	-1.948446	4.784610	1.054345
9	6	0	2.447851	-0.584124	-2.532801
10	6	0	2.396838	-2.622621	-0.586285
11	6	0	-3.181073	4.143510	0.389294
12	6	0	3.604407	-1.374945	-2.274123
13	6	0	3.586082	-2.371756	-1.320119
14	6	0	-3.906494	5.181756	-0.483236
15	6	0	-4.139960	3.570834	1.449830
16	1	0	-0.576353	1.664302	-3.227342
17	1	0	0.394611	-2.021903	-0.141157
18	1	0	-0.830554	-0.193789	-0.094092
19	1	0	-1.258565	5.168528	0.294153
20	1	0	1.537736	1.849539	-4.532029
21	1	0	-1.423246	4.057000	1.682020
22	1	0	-2.282144	5.617435	1.687456
23	1	0	-2.963600	3.166271	-1.528658
24	1	0	-3.228859	5.592351	-1.245323
25	1	0	-3.634891	2.805812	2.049571
26	1	0	-4.253000	6.007957	0.148514
27	1	0	4.494945	-1.181144	-2.868392
28	1	0	-4.466162	4.377284	2.119385
29	1	0	4.460645	-2.992247	-1.135949
30	1	0	-4.782615	4.737243	-0.977914
31	1	0	-5.027775	3.133969	0.971339
32	7	0	2.531172	0.363622	-3.511813
33	7	0	-2.771090	3.043488	-0.542599
34	8	0	-1.639542	1.678802	0.920954
35	8	0	-1.938911	1.104701	-1.289488
36	6	0	1.257232	-4.530093	0.332743
37	1	0	0.419858	-4.039014	0.843018
38	1	0	0.984210	-4.806039	-0.695914
39	1	0	1.555017	-5.430718	0.882774
40	8	0	2.440362	-3.680113	0.304656
41	6	0	-1.923581	-1.320711	-1.556264
42	6	0	-2.799561	-1.180305	-2.831327
43	6	0	-3.369392	-3.157990	-0.782709
44	6	0	-4.126385	-4.012517	-3.044582
45	6	0	-3.935921	-0.873453	-0.064245
46	6	0	-4.265393	-1.519301	-2.477587
47	6	0	-4.376792	-2.989991	-1.966273
48	6	0	-4.738452	-0.565221	-1.354669
49	6	0	-5.040702	-4.886465	-3.480113
50	1	0	-1.194678	-2.127671	-1.678217
51	1	0	-2.165869	-1.928149	0.447982
52	1	0	-2.424817	-1.850040	-3.612608
53	1	0	-2.517730	-3.794235	-1.048701
54	1	0	-2.743877	-0.156339	-3.214346
55	1	0	-3.124364	-4.015079	-3.482951
56	1	0	-3.504740	0.008062	0.409957
57	1	0	-3.842141	-3.568037	0.115362
58	1	0	-4.814894	-5.600121	-4.271072
59	1	0	-4.535911	-1.403002	0.684266
60	1	0	-4.571199	0.474074	-1.660575
61	1	0	-4.897510	-1.400658	-3.364327
62	1	0	-5.397337	-3.130328	-1.583819
63	1	0	-5.810431	-0.701429	-1.166872
64	1	0	-6.046037	-4.911161	-3.055957
65	7	0	-2.799309	-1.810308	-0.405231
66	6	0	-0.189346	-0.761980	3.210328
67	6	0	1.676181	1.907337	0.232041
68	6	0	1.793786	0.006378	1.967879
69	6	0	2.301803	2.613531	-0.798576
70	6	0	2.383327	0.890985	0.894101
71	6	0	3.612197	2.357850	-1.202834
72	6	0	3.709512	0.624325	0.516285
73	6	0	4.293757	1.354130	-0.516475
74	1	0	0.487542	-0.881888	4.061502
75	1	0	-0.125939	0.754665	1.717234
76	1	0	0.653934	2.165801	0.485237
77	1	0	4.072744	2.899217	-2.021981
78	1	0	4.269491	-0.157743	1.015991
79	7	0	0.475697	0.120801	2.239990
80	7	0	1.519816	3.652812	-1.535490
81	7	0	5.695874	1.018634	-0.939119
82	8	0	0.335026	3.797261	-1.220745
83	8	0	2.092369	4.281249	-2.418459
84	8	0	2.525243	-0.813679	2.556616
85	8	0	6.187406	1.690294	-1.839639
86	8	0	6.248847	0.084487	-0.360772
87	6	0	-0.419935	-2.179513	2.589968
88	8	0	0.074696	-3.164098	3.181934
89	8	0	-1.080450	-2.229655	1.496876

90	6	0	-0.386204	1.282743	5.478256
91	6	0	-1.516068	-0.145427	3.679866
92	6	0	-1.393652	1.256449	4.315566
93	6	0	-2.782077	1.720563	4.788718
94	1	0	0.632644	1.045956	5.140989
95	1	0	-0.363063	2.277140	5.945032
96	1	0	-0.672164	0.552763	6.251534
97	1	0	-1.046939	1.952507	3.537309
98	1	0	-1.951645	-0.838656	4.415955
99	1	0	-2.204364	-0.096874	2.824772
100	1	0	-2.743513	2.749332	5.173131
101	1	0	-3.147639	1.069178	5.597193
102	1	0	-3.513667	1.686967	3.968468
103	19	0	2.670146	-3.330127	3.167386

$1_R K^+$

E(RB97D) = -3156.53270074 A.U.
NImag = 0

Zero-point correction= 0.818995 (Hartree/Particle)
Thermal correction to Energy= 0.874129
Thermal correction to Enthalpy= 0.875073
Thermal correction to Gibbs Free Energy= 0.726861
Sum of electronic and zero-point Energies= -3155.713705
Sum of electronic and thermal Energies= -3155.658572
Sum of electronic and thermal Enthalpies= -3155.657628
Sum of electronic and thermal Free Energies= -3155.805840

E(RPBE1PBE) = -3155.00738416 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.194362	-0.896217	-3.170468
2	6	0	-0.294152	-0.038402	-2.089768
3	6	0	0.930517	0.312685	-1.254053
4	6	0	-1.342283	-1.196776	-3.949228
5	6	0	-1.575955	0.536505	-1.790905
6	6	0	-1.837752	1.395035	-0.688120
7	6	0	2.464567	-1.527656	-0.744347
8	6	0	-2.661076	0.188659	-2.679245
9	6	0	3.080058	-4.497317	-0.075146
10	6	0	-3.115960	1.910734	-0.491391
11	6	0	-3.944396	0.750373	-2.448728
12	6	0	4.055981	-3.492319	-0.714805
13	6	0	-4.174126	1.601656	-1.387313
14	6	0	4.847609	-4.173198	-1.844225
15	6	0	5.019293	-2.912270	0.338177
16	1	0	0.702049	0.195498	-0.187115
17	1	0	0.753564	-1.360928	-3.422130
18	1	0	-1.065844	1.622839	0.045136
19	1	0	-1.258116	-1.895061	-4.783929
20	1	0	2.369148	-4.873400	-0.820493
21	1	0	2.525139	-4.032080	0.746152
22	1	0	3.410810	-2.250251	-2.366381
23	1	0	3.656064	-5.341716	0.325790
24	1	0	4.167978	-4.583027	-2.605131
25	1	0	4.463099	-2.394518	1.127839
26	1	0	-4.746832	0.477419	-3.130284
27	1	0	-5.171764	1.999949	-1.234905
28	1	0	5.433292	-5.000716	-1.427369
29	1	0	5.542493	-3.465425	-2.319819
30	1	0	5.590003	-3.730897	0.795413
31	1	0	5.726945	-2.213700	-0.130111
32	7	0	-2.535935	-0.673466	-3.730826
33	7	0	3.301017	-2.371975	-1.367506
34	8	0	2.037371	-0.543598	-1.619347
35	8	0	2.152589	-1.557102	0.445173
36	6	0	-4.638545	3.192650	0.878048
37	1	0	-4.574663	3.777299	1.803495
38	1	0	-4.984030	3.846232	0.065105
39	1	0	-5.334133	2.352812	1.011741
40	8	0	-3.300371	2.712206	0.618145
41	6	0	1.336172	1.786862	-1.498003
42	6	0	2.152540	2.059970	-2.793796
43	6	0	2.305891	3.830743	-0.525371
44	6	0	2.792294	5.132287	-2.643743
45	6	0	3.297122	4.062501	-1.710687
46	6	0	3.441077	1.690384	-0.096273
47	6	0	3.473525	6.239496	-2.959311
48	6	0	3.514013	2.685130	-2.411175
49	6	0	4.242768	1.742103	-1.424288
50	1	0	0.407582	2.365149	-1.501361
51	1	0	1.316141	4.256723	-0.726904
52	1	0	1.479034	2.222137	0.579854
53	1	0	1.591351	2.734660	-3.449303
54	1	0	1.802678	4.965230	-3.078342
55	1	0	2.316631	1.126562	-3.341425
56	1	0	2.675045	4.243234	0.419022
57	1	0	3.070076	6.978877	-3.649620
58	1	0	3.256348	0.678051	0.265539
59	1	0	3.926003	2.257824	0.706314
60	1	0	4.120617	2.831977	-3.311445
61	1	0	4.266622	4.383639	-1.305156
62	1	0	4.313514	0.738331	-1.857642
63	1	0	4.459434	6.437296	-2.535006
64	1	0	5.258552	2.107817	-1.230981
65	7	0	2.099802	2.350298	-0.308168
66	6	0	-1.103231	-0.455218	2.184387
67	6	0	1.102141	0.273680	3.086294
68	6	0	-1.185281	-2.205612	0.283276
69	6	0	-1.816224	-1.282982	1.131425
70	6	0	-1.923746	-2.816410	-0.736284
71	6	0	-3.183491	-1.018392	0.950346
72	6	0	-3.275933	-2.554465	-0.949024
73	6	0	-3.881654	-1.646777	-0.077437
74	1	0	-0.135265	-2.463261	0.374530
75	1	0	0.744131	-1.109266	1.538015
76	1	0	2.109586	0.148382	2.664699
77	1	0	-3.682404	-0.310504	1.602057
78	1	0	-3.824967	-3.017514	-1.762041
79	7	0	0.240820	-0.542630	2.216081
80	7	0	-1.220426	-3.750527	-1.670927
81	7	0	-5.325745	-1.301465	-0.281939
82	8	0	0.007824	-3.821925	-1.575475
83	8	0	-1.757038	0.302911	2.924585
84	8	0	-1.901759	-4.368091	-2.480890
85	8	0	-5.820474	-0.469110	0.480183
86	8	0	-5.914670	-1.854967	-1.203449
87	6	0	0.750013	1.789284	2.944321
88	8	0	0.523550	2.210802	1.734680
89	8	0	0.650780	2.495764	3.958159
90	6	0	1.097988	-0.232200	4.537604
91	6	0	1.429641	-2.110335	6.177241
92	6	0	1.503381	-1.712066	4.692553
93	6	0	2.907642	-1.995191	4.125628
94	1	0	0.095644	-0.074188	4.956032
95	1	0	0.426489	-1.925207	6.587415
96	1	0	0.777005	-2.326478	4.135922
97	1	0	1.667586	-3.174998	6.311022
98	1	0	1.786455	0.403874	5.111203
99	1	0	2.151440	-1.523826	6.766174
100	1	0	2.954582	-1.831714	3.040035
101	1	0	3.198123	-3.037721	4.318321
102	1	0	3.652675	-1.343253	4.608852
103	19	0	-1.910603	2.989445	3.103320

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5. References

S1 Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
S2 E. D. Glendening, A. E. Reed, J. E. Carpenter, F. Weinhold, NBO; Version 3.1.