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

Supporting Information for

The Role of Alkali Metal Cations in the Stabilization of Guanine Quadruplexes: Why K^+ is the best.

F. Zaccaria,[a] G. Paragi,[a,b] C. Fonseca Guerra[a,*]

[a] Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling, Vrije Universiteit Amsterdam, De Boelelaan 1083, 1081 HV Amsterdam (The Netherlands).
[b] MTA-SZTE Supramolecular and Nanostructured Materials Research Group, Dóm tér 8, Szeged (Hungary)
E-mail: c.fonsecaguerra@vu.nl

Table S1 Solvation energies and radii of metal cations for COSMO computations.

Table S2 Preparation energy of the empty scaffold in the gas phase and in solution.

Table S3 Energy Decomposition Analysis for eight formaldehydes.

Figure S1 Top and side view of the $(H_2CO)_4$–$(H_2CO)_4$ stack.

Table S4. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of G_4-M^+-G_4 at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

Table S5. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of GQ-M^+ at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

Table S6 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of GQ_{4Na}-M^+ at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

Table S7. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of guanine, guanosine dimer (guanosine monophosphate + guanosine) and $(H_2CO)_8$ at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

Table S1. Solvation energies and radii of metal cations for COSMO computations.

	Experimental[a] ΔG_{hyd}	Ionic Radii Parameter in COSMO[b]	Computed solvation energy
Li^+	-113.4	1.4424	-113.4
Na^+	-87.2	1.8685	-87.4
K^+	-70.5	2.3350	-69.8
Rb^+	-65.7	2.4800	-65.7
Cs^+	-59.7	2.7225	-59.7

[a] Y. Marcus, *J. Chem. Soc., Faraday Trans.*, 1991, **87**, 2995–2999

[b] The solvation radii parameter in COSMO was adjusted in order to reproduce the experimental ΔG_{hyd} for the ZORA-BLYP-D3(BJ)/TZ2P level of theory.

Table S2 Preparation energy of the empty scaffold in the gas phase and in solution.[a]

System	M^+	$\Delta E_{prep,gas}$	$\Delta E_{prep,aq}$
G_4-M^+-G_4	Li^+	12.9	13.0
	Na^+	10.5	11.8
	K^+	5.5	5.3
	Rb^+	4.5	3.6
	Cs^+	6.2	4.1
GQ-M^+	Li^+	11.3	11.4
	Na^+	10.4	11.4
	K^+	5.7	5.1
	Rb^+	0.9	2.4
	Cs^+	1.8	1.8

[a] Energies and geometries computed at ZORA-BLYP-D3(BJ)/TZ2P level of theory.

Table S3 Energy Decomposition Analysis for eight formaldehydes.[a]

System	ΔE_{int}	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}	ΔE_{disp}
$[H_2CO]_8$	0.0	9.1	6.8	-5.7	-10.1
Pair (in same layer)	0.0	0.9	0.1	-0.3	-0.7
Diagonal (in same layer)	0.4	0.1	0.5	0.0	-0.1
Stack (on top of each other)	0.3	0.5	0.6	-0.2	-0.7
Stack far	0.0	0.2	0.3	-0.1	-0.3

[a] Energies and geometries computed at ZORA-BLYP-D3(BJ)/TZ2P level of theory.

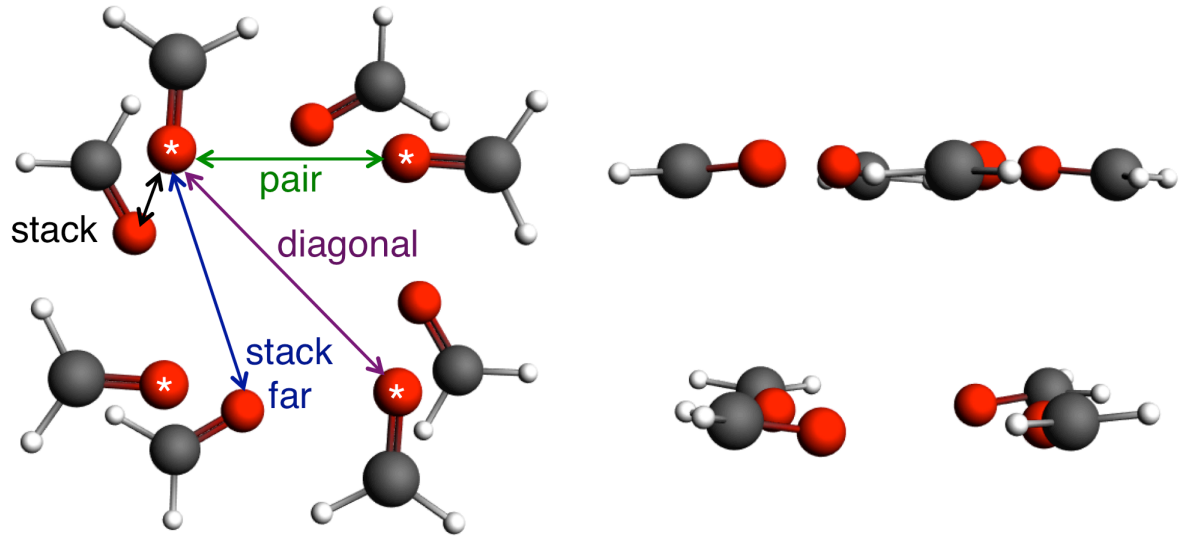

Figure S1 Top and side view of the $(H_2CO)_4$–$(H_2CO)_4$ stack. Oxygen atoms with a star are in the top layer.

Table S4. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of G_4-M^+-G_4 at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

G_4-**Li^+**-G_4 (Bond Energy: -19996.6 kcal/mol)			
1.C	3.083931	−4.693397	−1.623018
2.N	0.745807	−3.503633	−1.559221
3.H	−5.130921	1.211896	−1.664700
4.C	4.877418	0.848117	−1.641691
5.N	5.581231	−0.289278	−1.731759
6.H	−4.788408	5.981066	−1.674801
7.C	0.850549	−4.885194	−1.626408
8.N	5.517472	2.025200	−1.655818
9.H	6.234285	−3.884714	−1.633743
10.H	−0.180050	−3.038619	−1.528908
11.H	−1.219024	−5.134271	−1.631592
12.H	−0.207769	−6.595755	−1.643081
13.N	−0.287098	−5.589650	−1.708798
14.N	2.027567	−5.525080	−1.639391
15.C	4.686249	3.081813	−1.631540
16.H	−3.035736	0.172029	−1.541615
17.H	−6.593525	0.200723	−1.675430
18.N	−4.420047	5.037040	−1.652951
19.C	−5.158229	3.870820	−1.670881
20.N	−0.750286	3.494707	−1.543666
21.N	4.416256	−5.046587	−1.630519
22.H	5.126174	−1.221136	−1.651727
23.C	5.154929	−3.880515	−1.627870
24.N	−4.388108	2.798112	−1.655115
25.H	−5.989608	−4.791776	−1.649562
26.H	0.203671	6.587594	−1.612685
27.N	0.283510	5.581453	−1.676557
28.N	−2.031684	5.516205	−1.628341
29.C	−3.087911	4.684063	−1.629987
30.C	−3.079765	3.278076	−1.624454
31.C	−1.830587	2.602521	−1.565768
32.O	−1.624317	1.356418	−1.532374
33.H	6.587487	−0.210316	−1.667008
34.N	3.496280	0.743778	−1.565817
35.H	1.215712	5.125598	−1.603674
36.N	4.384863	−2.807734	−1.617562
37.C	3.076147	−3.287453	−1.607912
38.C	3.873957	5.152925	−1.628581
39.N	2.800984	4.383205	−1.612051
40.C	3.280422	3.074356	−1.607383
41.C	2.604787	1.824772	−1.560718
42.N	−5.045421	−4.423805	−1.631680
43.C	−3.879508	−5.162686	−1.630444
44.N	−2.806460	−4.393023	−1.621554
45.C	−3.285908	−3.084175	−1.613322
46.C	−2.610062	−1.834624	−1.569526
47.H	5.983767	4.782004	−1.666351
48.O	−1.364110	−1.628679	−1.531446
49.N	−3.501424	−0.753494	−1.571696
50.C	−4.883021	−0.857889	−1.640551
51.N	−5.586740	0.279285	−1.729752
52.N	−5.523180	−2.034981	−1.647854
53.O	1.620360	−1.365800	−1.525035
54.C	−0.854460	4.876533	−1.607071
55.H	3.878305	6.232387	−1.632934
56.C	−4.691832	−3.091676	−1.627639
57.H	−3.884361	−6.242164	−1.636058
58.C	1.826475	−2.611765	−1.562156
59.N	5.039821	4.414002	−1.638322
60.O	1.359027	1.618933	−1.517710
61.H	−6.237397	3.874632	−1.693270
62.H	0.175086	3.029074	−1.506403

63.H	4.784839	−5.990623	−1.649612
64.H	3.030886	−0.181890	−1.533030
65.C	5.420601	−1.813370	1.614335
66.N	2.822171	−2.214305	1.610570
67.H	−4.743614	−2.194426	1.627189
68.C	3.281462	3.718896	1.674569
69.N	4.528681	3.210826	1.749276
70.H	−7.558060	1.873935	1.591211
71.C	3.712888	−3.270007	1.671681
72.N	3.116965	5.049345	1.684334
73.H	7.502743	0.688654	1.543614
74.H	1.796452	−2.395020	1.589704
75.H	2.198179	−4.739089	1.642860
76.H	3.868756	−5.274821	1.680281
77.N	3.204070	−4.515712	1.758135
78.N	5.043701	−3.106628	1.676524
79.C	1.822771	5.425356	1.635455
80.H	−2.398834	−1.792157	1.588063
81.H	−5.279335	−3.864355	1.663484
82.N	−6.704827	1.327200	1.567553
83.C	−6.618838	−0.053674	1.547629
84.N	−2.818825	2.225257	1.604387
85.N	6.708737	−1.318737	1.594324
86.H	4.751619	2.205823	1.625411
87.C	6.623819	0.061956	1.560480
88.N	−5.364742	−0.471463	1.551635
89.H	−1.871029	−7.556519	1.630912
90.H	−3.867308	5.286147	1.650138
91.N	−3.203474	4.527100	1.735131
92.N	−5.041403	3.116670	1.648873
93.C	−5.417067	1.822820	1.592256
94.C	−4.592681	0.688488	1.568799
95.C	−3.180152	0.862210	1.575990
96.O	−2.294358	−0.022269	1.565178
97.H	5.286355	3.875964	1.660620
98.N	2.225949	2.827494	1.621088
99.H	−2.195759	4.749782	1.637710
100.N	5.370012	0.480672	1.553402
101.C	4.597135	−0.678652	1.577156
102.C	−0.053606	6.627443	1.603623
103.N	−0.471715	5.373361	1.600538
104.C	0.688309	4.601169	1.609473
105.C	0.862280	3.188587	1.607022
106.N	−1.323383	−6.704196	1.601594
107.C	0.057567	−6.619772	1.577814
108.N	0.476531	−5.366097	1.574767
109.C	−0.682726	−4.592903	1.591634
110.C	−0.855499	−3.180153	1.593364
111.H	1.874092	7.566144	1.647722
112.O	0.029022	−2.294698	1.582464
113.N	−2.218662	−2.817723	1.614582
114.C	−3.274714	−3.708316	1.670333
115.N	−4.521174	−3.199636	1.750231
116.N	−3.111293	−5.038943	1.676723
117.O	2.299429	0.033441	1.555096
118.C	−3.710581	3.280762	1.653618
119.H	−0.680918	7.506088	1.593746
120.C	−1.817760	−5.415936	1.620892
121.H	0.683960	−7.499035	1.564798
122.C	3.184486	−0.851559	1.576676
123.N	1.327197	6.713160	1.621652
124.O	−0.021820	2.302475	1.599532
125.H	−7.497210	−0.681198	1.532486
126.H	−1.793195	2.406049	1.590864
127.H	7.561525	−1.865871	1.623573
128.H	2.407071	1.802179	1.588900
129.Li	−0.002946	−0.003757	−1.265952

G_4-**Na^+**-G_4 (Bond Energy: -19988.6 kcal/mol)

1.O	−0.519355	−2.168369	1.444623
2.N	−2.823925	−2.203686	1.583610
3.C	−4.045170	−2.847262	1.688656
4.N	−4.166031	−4.181638	1.729544
5.C	−2.984963	−4.824983	1.661038
6.C	−1.701000	−4.261508	1.583042
7.C	−1.574589	−2.846963	1.530114
8.N	−2.776471	−6.188322	1.666738
9.C	−1.411488	−6.400633	1.606167
10.N	−0.735660	−5.266206	1.557482
11.H	−5.139222	−1.050727	1.651771
12.H	−6.036253	−2.565368	1.744554
13.H	−2.776599	−1.165483	1.542042
14.H	−3.492317	−6.903363	1.728378
15.H	−0.985637	−7.392713	1.603656
16.N	−2.096057	5.158168	1.751614
17.O	−2.184213	0.526588	1.469158
18.N	−2.218821	2.832347	1.585207
19.C	−2.862218	4.054984	1.677465
20.N	−4.196193	4.176567	1.717570
21.C	−4.839807	2.995121	1.661590
22.C	−4.276877	1.710241	1.596446
23.C	−2.862628	1.582581	1.544579
24.N	−6.203086	2.787147	1.668177
25.C	−6.415937	1.421678	1.621320
26.N	−5.281724	0.745097	1.579096
27.H	−1.064539	5.144806	1.632017
28.H	−2.578856	6.046518	1.711025
29.H	−1.181857	2.784832	1.536338
30.H	−6.917762	3.503918	1.722254
31.H	−7.408449	0.996733	1.621810
32.N	5.144535	2.093746	1.798931
33.O	0.518208	2.176831	1.432400
34.N	2.821381	2.214913	1.593480
35.C	4.041198	2.859237	1.709809
36.N	4.159884	4.192925	1.759732
37.C	2.978680	4.835208	1.686989
38.C	1.695640	4.270741	1.596788
39.C	1.572196	2.856835	1.534041
40.N	2.769191	6.198085	1.694670
41.C	1.404888	6.409665	1.621435
42.N	0.730150	5.275027	1.563674
43.H	5.136035	1.065988	1.648047
44.H	6.031742	2.579412	1.766188
45.H	2.776604	1.177468	1.542168
46.H	3.484134	6.913721	1.759653
47.H	0.978949	7.401705	1.614651
48.N	2.089329	−5.140696	1.781296
49.O	2.170821	−0.514025	1.426730
50.N	2.208838	−2.817430	1.581685
51.C	2.854215	−4.037807	1.690062
52.N	4.188501	−4.156871	1.729017
53.C	4.830207	−2.975916	1.651516
54.C	4.264951	−1.692866	1.566814
55.C	2.850942	−1.569188	1.517813
56.N	6.193162	−2.765690	1.651537
57.C	6.403565	−1.400858	1.580199
58.N	5.268451	−0.726631	1.530892
59.H	1.059192	−5.131448	1.648805
60.H	2.574146	−6.028397	1.752910
61.H	1.170787	−2.771606	1.536328
62.H	6.909368	−3.480501	1.710878
63.H	7.395410	−0.974562	1.569408
64.N	−5.148058	−2.081876	1.775272
65.N	−1.768380	−5.285688	−1.702126
66.O	1.300860	−1.813235	−1.474117
67.N	−0.167662	−3.593517	−1.560010

68.C	−0.470976	−4.942803	−1.633201
69.N	0.467325	−5.900437	−1.658536
70.C	1.723569	−5.415809	−1.633729
71.C	2.126941	−4.070768	−1.601581
72.C	1.131750	−3.058863	−1.542458
73.N	2.897305	−6.140596	−1.639237
74.C	3.943654	−5.237356	−1.620116
75.N	3.518610	−3.986673	−1.598220
76.H	−2.545315	−4.601737	−1.621235
77.H	−1.979933	−6.273875	−1.659208
78.H	−0.926049	−2.884002	−1.519705
79.H	2.977845	−7.150607	−1.669188
80.H	4.974851	−5.556838	−1.623408
81.N	−5.286217	1.761488	−1.674565
82.O	−1.818184	−1.314049	−1.490943
83.N	−3.596417	0.157616	−1.551364
84.C	−4.945946	0.463591	−1.617645
85.N	−5.904962	−0.473535	−1.645188
86.C	−5.422013	−1.730972	−1.629345
87.C	−4.077896	−2.136374	−1.602450
88.C	−3.063219	−1.143479	−1.545817
89.N	−6.148466	−2.903606	−1.643407
90.C	−5.246497	−3.951508	−1.631938
91.N	−3.995277	−3.527937	−1.608601
92.H	−4.597300	2.535731	−1.612660
93.H	−6.273959	1.976496	−1.643566
94.H	−2.885910	0.913356	−1.508228
95.H	−7.158585	−2.982732	−1.672850
96.H	−5.566665	−4.982342	−1.643268
97.N	1.776483	5.277963	−1.692345
98.O	−1.287535	1.801555	−1.458396
99.N	0.177249	3.584574	−1.551631
100.C	0.479129	4.933905	−1.632959
101.N	−0.460795	5.888972	−1.674636
102.C	−1.716374	5.401927	−1.656418
103.C	−2.117779	4.056568	−1.612562
104.C	−1.121528	3.046611	−1.537713
105.N	−2.890902	6.124670	−1.679829
106.C	−3.936032	5.220180	−1.656297
107.N	−3.509149	3.970520	−1.616877
108.H	2.551726	4.593417	−1.600140
109.H	1.986906	6.266732	−1.656860
110.H	0.935781	2.877511	−1.504298
111.H	−2.972378	7.134053	−1.722880
112.H	−4.967812	5.537238	−1.670878
113.N	5.293995	−1.777674	−1.727910
114.O	1.819488	1.282999	−1.449215
115.N	3.601516	−0.180215	−1.565181
116.C	4.950778	−0.481043	−1.651801
117.N	5.906061	0.459036	−1.681174
118.C	5.419943	1.714153	−1.640427
119.C	4.074453	2.114967	−1.588623
120.C	3.065452	1.117541	−1.530669
121.N	6.142611	2.888950	−1.643177
122.C	5.238165	3.933565	−1.599710
123.N	3.988459	3.506271	−1.567657
124.H	4.608704	−2.552461	−1.637681
125.H	6.282707	−1.988981	−1.696804
126.H	2.893188	−0.938930	−1.525855
127.H	7.152260	2.971267	−1.678861
128.H	5.555354	4.965377	−1.594602
129.Na	0.079067	0.039299	−0.094328

G_4-$\mathbf{K^+}$-G_4 (Bond Energy: -19991.3 kcal/mol)			
1.O	−0.260682	−2.271941	1.591501
2.N	−2.550943	−2.559223	1.601161
3.C	−3.699109	−3.332788	1.645837

4.N	−3.673129	−4.673430	1.635583
5.C	−2.425149	−5.184170	1.629599
6.C	−1.208522	−4.482298	1.642608
7.C	−1.237560	−3.064237	1.614747
8.N	−2.065579	−6.515444	1.622696
9.C	−0.683498	−6.573929	1.642332
10.N	−0.134780	−5.372200	1.657027
11.H	−4.980857	−1.661875	1.664887
12.H	−5.709319	−3.262787	1.659921
13.H	−2.624892	−1.523644	1.594920
14.H	−2.698293	−7.307345	1.624744
15.H	−0.152462	−7.513798	1.645759
16.N	−2.696825	4.877877	1.705401
17.O	−2.276627	0.260332	1.584865
18.N	−2.564485	2.550519	1.584381
19.C	−3.338108	3.698514	1.628013
20.N	−4.678815	3.672193	1.624263
21.C	−5.189291	2.424123	1.627518
22.C	−4.487010	1.207712	1.642572
23.C	−3.069194	1.236988	1.607139
24.N	−6.520491	2.064264	1.629826
25.C	−6.578264	0.682317	1.658498
26.N	−5.376460	0.133922	1.668937
27.H	−1.667404	4.981671	1.636891
28.H	−3.268956	5.709261	1.635388
29.H	−1.528907	2.624401	1.576680
30.H	−7.312626	2.696628	1.632906
31.H	−7.518004	0.151165	1.670344
32.N	4.871928	2.698447	1.728609
33.O	0.255088	2.276599	1.584024
34.N	2.545214	2.564982	1.596017
35.C	3.692906	3.339243	1.640304
36.N	3.666135	4.679814	1.627179
37.C	2.417918	5.189881	1.617795
38.C	1.201675	4.487417	1.630034
39.C	1.231566	3.069369	1.606483
40.N	2.057729	6.521056	1.606213
41.C	0.675547	6.578656	1.622507
42.N	0.127467	5.376770	1.639360
43.H	4.975729	1.669161	1.661577
44.H	5.703429	3.270140	1.656151
45.H	2.619372	1.529471	1.591867
46.H	2.689758	7.313454	1.606041
47.H	0.144014	7.518209	1.619501
48.N	2.689045	−4.872108	1.729429
49.O	2.270077	−0.254598	1.594253
50.N	2.556903	−2.544862	1.604406
51.C	3.330345	−3.692855	1.647588
52.N	4.671134	−3.666933	1.640252
53.C	5.181964	−2.418881	1.637876
54.C	4.480074	−1.202426	1.650768
55.C	3.062079	−1.231595	1.619272
56.N	6.513259	−2.059349	1.633762
57.C	6.571707	−0.677204	1.654137
58.N	5.369901	−0.128575	1.666504
59.H	1.659848	−4.975691	1.657271
60.H	3.260550	−5.703469	1.653861
61.H	1.521227	−2.618747	1.595067
62.H	7.305084	−2.692123	1.639494
63.H	7.511559	−0.146375	1.657656
64.N	−4.877747	−2.691270	1.732126
65.N	−2.362374	−5.037576	−1.765891
66.O	1.136175	−1.992357	−1.618773
67.N	−0.552171	−3.565130	−1.653186
68.C	−1.028841	−4.865036	−1.683037
69.N	−0.224664	−5.936470	−1.663335
70.C	1.084505	−5.620902	−1.611513
71.C	1.660752	−4.340095	−1.604254
72.C	0.807664	−3.206549	−1.625017

73.N	2.153825	−6.490312	−1.570109
74.C	3.309481	−5.728932	−1.555927
75.N	3.051270	−4.433114	−1.578338
76.H	−3.048916	−4.268275	−1.655178
77.H	−2.697064	−5.987486	−1.665852
78.H	−1.219436	−2.768762	−1.661258
79.H	2.103768	−7.502741	−1.577929
80.H	4.290247	−6.180112	−1.531216
81.N	−5.033270	2.362533	−1.764835
82.O	−1.985915	−1.134848	−1.640837
83.N	−3.559525	0.552857	−1.660697
84.C	−4.859764	1.029252	−1.680277
85.N	−5.930691	0.225016	−1.647657
86.C	−5.614322	−1.083909	−1.596674
87.C	−4.333410	−1.660055	−1.603690
88.C	−3.200533	−0.806734	−1.635919
89.N	−6.482984	−2.153366	−1.545276
90.C	−5.721363	−3.308903	−1.538903
91.N	−4.425929	−3.050556	−1.575835
92.H	−4.262791	3.049506	−1.665998
93.H	−5.982218	2.697498	−1.656942
94.H	−2.763165	1.219979	−1.673632
95.H	−7.495359	−2.103029	−1.541009
96.H	−6.171931	−4.289555	−1.507360
97.N	2.369539	5.031438	−1.771852
98.O	−1.129137	1.986053	−1.642137
99.N	0.558929	3.559043	−1.664893
100.C	1.035722	4.858776	−1.695217
101.N	0.231533	5.930268	−1.679937
102.C	−1.077705	5.614689	−1.632191
103.C	−1.654031	4.333893	−1.627740
104.C	−0.800776	3.200585	−1.645584
105.N	−2.147042	6.484080	−1.592512
106.C	−3.302661	5.722774	−1.579959
107.N	−3.044552	4.426953	−1.603758
108.H	3.055492	4.261741	−1.661805
109.H	2.703633	5.981246	−1.669135
110.H	1.226393	2.762987	−1.665297
111.H	−2.096706	7.496441	−1.597454
112.H	−4.283182	6.173948	−1.553349
113.N	5.038877	−2.368275	−1.750074
114.O	1.993960	1.130300	−1.624073
115.N	3.567126	−0.557716	−1.646565
116.C	4.866986	−1.034482	−1.674095
117.N	5.938480	−0.230252	−1.656035
118.C	5.622593	1.078908	−1.608048
119.C	4.341742	1.655131	−1.604880
120.C	3.208476	0.801932	−1.625549
121.N	6.491846	2.148497	−1.569116
122.C	5.730263	3.304100	−1.558944
123.N	4.434583	3.045679	−1.582946
124.H	4.267978	−3.053416	−1.644618
125.H	5.988588	−2.703494	−1.651275
126.H	2.771408	−1.225452	−1.651203
127.H	7.504253	2.098368	−1.575852
128.H	6.181168	4.284791	−1.534044
129.K	−0.001878	0.001285	−0.027099

G_4-**Rb^+**-G_4 (Bond Energy: -19985.1 kcal/mol)			
1.O	−0.186951	−2.305965	1.712213
2.N	−2.470739	−2.639038	1.654121
3.C	−3.603549	−3.436043	1.659669
4.N	−3.549537	−4.775626	1.631100
5.C	−2.291095	−5.261523	1.644983
6.C	−1.089356	−4.535341	1.688331
7.C	−1.147136	−3.118599	1.690934
8.N	−1.903428	−6.584429	1.634852

9.C	−0.520896	−6.614206	1.681884
10.N	0.003029	−5.401918	1.718485
11.H	−4.926464	−1.793756	1.670434
12.H	−5.614983	−3.408645	1.634240
13.H	−2.571994	−1.606112	1.675924
14.H	−2.518754	−7.389760	1.616972
15.H	0.028959	−7.543148	1.687367
16.N	−2.824440	4.799513	1.737046
17.O	−2.313798	0.189133	1.699120
18.N	−2.645120	2.472934	1.653506
19.C	−3.440963	3.606494	1.658740
20.N	−4.780274	3.553657	1.618842
21.C	−5.267397	2.295506	1.623709
22.C	−4.542692	1.092866	1.669907
23.C	−3.126051	1.149658	1.680573
24.N	−6.590375	1.908982	1.600201
25.C	−6.622052	0.526346	1.642144
26.N	−5.410524	0.001121	1.687940
27.H	−1.797805	4.928444	1.685600
28.H	−3.410874	5.617952	1.637863
29.H	−1.612178	2.572390	1.679024
30.H	−7.395041	2.524897	1.576511
31.H	−7.551462	−0.022697	1.635332
32.N	4.794442	2.828768	1.733414
33.O	0.184165	2.316632	1.703158
34.N	2.468189	2.648317	1.647859
35.C	3.601162	3.445041	1.657318
36.N	3.547745	4.784474	1.623356
37.C	2.289504	5.270913	1.631016
38.C	1.087542	4.545256	1.676173
39.C	1.144949	3.128740	1.681771
40.N	1.902010	6.593846	1.614806
41.C	0.519394	6.624101	1.658479
42.N	−0.004793	5.412034	1.699825
43.H	4.923867	1.802475	1.678560
44.H	5.612681	3.416332	1.640408
45.H	2.568851	1.615474	1.672765
46.H	2.516890	7.399244	1.589698
47.H	−0.030342	7.553141	1.655034
48.N	2.823193	−4.791063	1.742718
49.O	2.311353	−0.181061	1.709421
50.N	2.643303	−2.464987	1.657989
51.C	3.439969	−3.598288	1.666546
52.N	4.779356	−3.544796	1.630699
53.C	5.265530	−2.286405	1.633588
54.C	4.540192	−1.084019	1.675655
55.C	3.123669	−1.141514	1.687873
56.N	6.588411	−1.899281	1.612418
57.C	6.619163	−0.516466	1.650724
58.N	5.407385	0.008258	1.692807
59.H	1.796470	−4.919483	1.694927
60.H	3.410063	−5.609981	1.651572
61.H	1.610430	−2.565339	1.683500
62.H	7.393340	−2.514980	1.593715
63.H	7.548486	0.032715	1.643207
64.N	−4.797340	−2.819945	1.725079
65.N	−2.489687	−4.988047	−1.739585
66.O	1.106983	−2.054806	−1.863360
67.N	−0.633026	−3.569264	−1.752910
68.C	−1.150062	−4.852376	−1.677372
69.N	−0.379129	−5.943171	−1.578379
70.C	0.939911	−5.666247	−1.556944
71.C	1.555507	−4.407787	−1.654070
72.C	0.738904	−3.254304	−1.766707
73.N	1.982773	−6.561955	−1.452890
74.C	3.161310	−5.837436	−1.505259
75.N	2.942995	−4.539865	−1.628097
76.H	−3.151692	−4.193976	−1.676651
77.H	−2.852250	−5.914152	−1.551531

78.H	−1.279740	−2.760652	−1.822530
79.H	1.902828	−7.570117	−1.383521
80.H	4.127709	−6.315525	−1.449394
81.N	−4.985291	2.486739	−1.773665
82.O	−2.048928	−1.108298	−1.868094
83.N	−3.565149	0.631026	−1.766851
84.C	−4.849458	1.147013	−1.704781
85.N	−5.940200	0.375446	−1.613114
86.C	−5.662201	−0.943380	−1.584502
87.C	−4.402238	−1.558098	−1.667051
88.C	−3.248898	−0.740853	−1.776743
89.N	−6.557609	−1.986489	−1.483197
90.C	−5.831784	−3.164526	−1.524464
91.N	−4.533209	−2.945609	−1.636301
92.H	−4.192354	3.148385	−1.694471
93.H	−5.913281	2.848400	−1.592867
94.H	−2.756412	1.278053	−1.834917
95.H	−7.566520	−1.906902	−1.425604
96.H	−6.309645	−4.131054	−1.467298
97.N	2.492203	4.978511	−1.765101
98.O	−1.103872	2.044192	−1.886116
99.N	0.635489	3.558937	−1.772264
100.C	1.152137	4.842149	−1.698992
101.N	0.381092	5.932627	−1.600326
102.C	−0.937836	5.655203	−1.574577
103.C	−1.553377	4.396492	−1.668883
104.C	−0.736517	3.243459	−1.785523
105.N	−1.980613	6.550297	−1.464606
106.C	−3.158972	5.825205	−1.510395
107.N	−2.940827	4.527713	−1.634953
108.H	3.153986	4.185384	−1.690834
109.H	2.853322	5.904096	−1.571122
110.H	1.281792	2.749463	−1.840356
111.H	−1.900896	7.558402	−1.394226
112.H	−4.125213	6.302429	−1.445926
113.N	4.981518	−2.496298	−1.765455
114.O	2.051994	1.103756	−1.870765
115.N	3.564703	−0.637844	−1.764747
116.C	4.847755	−1.156570	−1.698729
117.N	5.939750	−0.386788	−1.603985
118.C	5.664244	0.932479	−1.577859
119.C	4.406060	1.549922	−1.667704
120.C	3.251353	0.734578	−1.777704
121.N	6.561343	1.973769	−1.472761
122.C	5.838129	3.153437	−1.516753
123.N	4.539768	2.937249	−1.635891
124.H	4.188054	−3.158307	−1.691574
125.H	5.909262	−2.859536	−1.586551
126.H	2.754210	−1.283272	−1.827856
127.H	7.569439	1.891717	−1.406124
128.H	6.317763	4.118874	−1.456718
129.Rb	0.000140	0.002458	−0.087358

G_4-**Cs**$^+$-G_4 (Bond Energy: -19977.9 kcal/mol)			
1.O	−0.216326	−2.333834	2.093321
2.N	−2.500320	−2.610809	1.873920
3.C	−3.643414	−3.382340	1.736635
4.N	−3.608301	−4.715270	1.600748
5.C	−2.360803	−5.226099	1.641750
6.C	−1.151772	−4.530501	1.807334
7.C	−1.187583	−3.120046	1.941929
8.N	−1.993934	−6.551457	1.545002
9.C	−0.616520	−6.612448	1.659305
10.N	−0.075653	−5.418141	1.822715
11.H	−4.940992	−1.719380	1.770405
12.H	−5.646143	−3.311447	1.570234
13.H	−2.589675	−1.582304	1.976971
14.H	−2.619682	−7.340916	1.432712

15.H	−0.082685	−7.549524	1.613123
16.N	−2.749776	4.840252	1.790726
17.O	−2.337652	0.224869	2.082191
18.N	−2.613605	2.509890	1.876394
19.C	−3.384534	3.654205	1.746085
20.N	−4.717225	3.620538	1.608917
21.C	−5.228452	2.372860	1.639745
22.C	−4.533480	1.162532	1.797812
23.C	−3.123391	1.197193	1.935643
24.N	−6.553525	2.006748	1.535267
25.C	−6.614835	0.628388	1.639026
26.N	−5.421064	0.086357	1.802191
27.H	−1.720465	4.949905	1.785802
28.H	−3.312198	5.658478	1.595952
29.H	−1.585608	2.598254	1.982236
30.H	−7.342330	2.633296	1.422682
31.H	−7.551494	0.094700	1.584537
32.N	4.840695	2.758261	1.777840
33.O	0.226084	2.345824	2.088585
34.N	2.510444	2.621295	1.871167
35.C	3.653928	3.392106	1.733118
36.N	3.619287	4.724117	1.590080
37.C	2.371699	5.235476	1.627125
38.C	1.162432	4.541176	1.796322
39.C	1.197699	3.131126	1.936231
40.N	2.005237	6.560205	1.520956
41.C	0.627737	6.622071	1.633838
42.N	0.086419	5.428988	1.804535
43.H	4.951998	1.728877	1.776374
44.H	5.657599	3.320936	1.578477
45.H	2.599138	1.592842	1.976375
46.H	2.631495	7.348567	1.404112
47.H	0.094088	7.558769	1.578506
48.N	2.757857	−4.829792	1.800770
49.O	2.346479	−0.213496	2.083450
50.N	2.621563	−2.498834	1.880939
51.C	3.392270	−3.643493	1.752884
52.N	4.725042	−3.610386	1.616383
53.C	5.236907	−2.362948	1.647785
54.C	4.542429	−1.152156	1.804144
55.C	3.132123	−1.186222	1.939916
56.N	6.562237	−1.997665	1.545348
57.C	6.624394	−0.619311	1.648323
58.N	5.430614	−0.076425	1.809100
59.H	1.728409	−4.941683	1.796675
60.H	3.321497	−5.647828	1.609032
61.H	1.592971	−2.586044	1.985020
62.H	7.350656	−2.625032	1.435060
63.H	7.561579	−0.086485	1.594307
64.N	−4.830203	−2.748610	1.772939
65.N	−2.422417	−5.024298	−1.743639
66.O	1.141869	−2.059338	−2.025497
67.N	−0.581826	−3.584123	−1.821658
68.C	−1.084101	−4.868585	−1.683441
69.N	−0.300772	−5.943234	−1.529823
70.C	1.014702	−5.650024	−1.513591
71.C	1.616314	−4.390490	−1.669642
72.C	0.787695	−3.255168	−1.855917
73.N	2.067412	−6.526260	−1.357987
74.C	3.237351	−5.790580	−1.436128
75.N	3.004795	−4.503305	−1.625788
76.H	−3.094699	−4.237921	−1.692760
77.H	−2.769860	−5.944985	−1.505881
78.H	−1.238201	−2.789293	−1.934960
79.H	1.998661	−7.531023	−1.242739
80.H	4.208978	−6.252923	−1.347476
81.N	−5.027368	2.412930	−1.752214
82.O	−2.056602	−1.148303	−2.015266
83.N	−3.585514	0.573899	−1.825507

84.C	−4.871371	1.074645	−1.696450
85.N	−5.946752	0.289871	−1.553910
86.C	−5.652178	−1.025506	−1.537282
87.C	−4.390253	−1.625213	−1.680840
88.C	−3.254381	−0.795156	−1.856256
89.N	−6.528299	−2.079702	−1.391605
90.C	−5.790315	−3.248440	−1.463049
91.N	−4.501522	−3.013902	−1.639211
92.H	−4.242059	3.085719	−1.696707
93.H	−5.951160	2.759864	−1.526376
94.H	−2.791340	1.231922	−1.935665
95.H	−7.534349	−2.013757	−1.289186
96.H	−6.253272	−4.220222	−1.379099
97.N	2.411182	5.011898	−1.767286
98.O	−1.156014	2.048009	−2.028238
99.N	0.569271	3.572539	−1.833661
100.C	1.072770	4.857286	−1.703352
101.N	0.290361	5.932978	−1.553035
102.C	−1.025321	5.640566	−1.531767
103.C	−1.628212	4.380771	−1.679928
104.C	−0.800764	3.244288	−1.863839
105.N	−2.076563	6.518497	−1.377120
106.C	−3.247320	5.783200	−1.447294
107.N	−3.016486	4.494837	−1.631687
108.H	3.083302	4.225650	−1.711776
109.H	2.759321	5.933661	−1.534507
110.H	1.225584	2.777963	−1.949284
111.H	−2.005984	7.523900	−1.268890
112.H	−4.218269	6.246049	−1.355097
113.N	5.014306	−2.423033	−1.743674
114.O	2.049065	1.140429	−2.040177
115.N	3.574245	−0.582766	−1.829693
116.C	4.858784	−1.084386	−1.690583
117.N	5.933677	−0.300266	−1.542341
118.C	5.640056	1.015213	−1.530457
119.C	4.380156	1.615930	−1.686173
120.C	3.244917	0.786563	−1.869227
121.N	6.516116	2.068710	−1.379057
122.C	5.779847	3.238271	−1.459033
123.N	4.492532	3.004549	−1.646707
124.H	4.227886	−3.094809	−1.689020
125.H	5.935457	−2.769780	−1.506488
126.H	2.780147	−1.240265	−1.942284
127.H	7.520595	2.000502	−1.262055
128.H	6.241851	4.210157	−1.371398
129.Cs	0.002902	0.006176	0.021379

G_4-[]-G_4 (Bond Energy: -19967.7 kcal/mol)			
1.O	−0.165011	−2.345307	1.843325
2.N	−2.448386	−2.632184	1.645960
3.C	−3.588319	−3.412411	1.604964
4.N	−3.557326	−4.751895	1.536453
5.C	−2.305377	−5.257661	1.559656
6.C	−1.097255	−4.553489	1.657808
7.C	−1.129117	−3.131560	1.720497
8.N	−1.939514	−6.587950	1.531153
9.C	−0.560153	−6.641887	1.621487
10.N	−0.020949	−5.438255	1.706570
11.H	−4.906477	−1.761154	1.645797
12.H	−5.595837	−3.362727	1.512121
13.H	−2.532127	−1.595025	1.669178
14.H	−2.567267	−7.381402	1.475344
15.H	−0.024539	−7.579128	1.619172
16.N	−2.792622	4.779605	1.697525
17.O	−2.348588	0.162651	1.815125
18.N	−2.637635	2.447607	1.640369
19.C	−3.418266	3.587777	1.619186

20.N	−4.758775	3.557294	1.568490
21.C	−5.264042	2.305037	1.590160
22.C	−4.558741	1.096276	1.670046
23.C	−3.135981	1.127779	1.712116
24.N	−6.594708	1.939022	1.574572
25.C	−6.647226	0.558621	1.655400
26.N	−5.442563	0.019260	1.720530
27.H	−1.766411	4.906142	1.645892
28.H	−3.370743	5.596322	1.547882
29.H	−1.599823	2.530589	1.651955
30.H	−7.389244	2.566805	1.534252
31.H	−7.584387	0.022857	1.659670
32.N	4.771837	2.792865	1.690905
33.O	0.154338	2.348862	1.776631
34.N	2.440180	2.638121	1.620574
35.C	3.580563	3.418623	1.605846
36.N	3.550562	4.758977	1.555569
37.C	2.298214	5.264661	1.572995
38.C	1.088996	4.559572	1.646552
39.C	1.119658	3.136606	1.684021
40.N	1.932524	6.595414	1.559761
41.C	0.551900	6.648106	1.635256
42.N	0.012050	5.443430	1.695749
43.H	4.898203	1.766772	1.640904
44.H	5.589569	3.370632	1.545884
45.H	2.522762	1.600868	1.641173
46.H	2.560062	7.390245	1.523849
47.H	0.016336	7.585392	1.638378
48.N	2.784621	−4.773818	1.697522
49.O	2.341519	−0.156160	1.812102
50.N	2.629184	−2.441574	1.643101
51.C	3.409662	−3.581861	1.616400
52.N	4.749672	−3.551531	1.556942
53.C	5.255324	−2.299336	1.573688
54.C	4.550729	−1.090261	1.654726
55.C	3.128228	−1.121462	1.706740
56.N	6.585970	−1.933773	1.551129
57.C	6.639405	−0.553395	1.628760
58.N	5.435194	−0.013470	1.699321
59.H	1.758457	−4.900606	1.651056
60.H	3.362141	−5.590298	1.544304
61.H	1.591940	−2.524751	1.670939
62.H	7.380061	−2.561787	1.507715
63.H	7.576848	−0.018113	1.626644
64.N	−4.781037	−2.787820	1.682501
65.N	−2.455422	−4.959441	−1.775509
66.O	1.163437	−2.057674	−1.998144
67.N	−0.591810	−3.542647	−1.769504
68.C	−1.113635	−4.820003	−1.685786
69.N	−0.353703	−5.917076	−1.569450
70.C	0.967817	−5.647657	−1.536785
71.C	1.591879	−4.398140	−1.655022
72.C	0.785429	−3.235219	−1.813852
73.N	2.003485	−6.552875	−1.423524
74.C	3.187983	−5.840325	−1.495291
75.N	2.977427	−4.543338	−1.640613
76.H	−3.121043	−4.170072	−1.695711
77.H	−2.812254	−5.877558	−1.541526
78.H	−1.232362	−2.724246	−1.829854
79.H	1.914331	−7.559138	−1.341711
80.H	4.150971	−6.324774	−1.434796
81.N	−4.953798	2.455669	−1.742633
82.O	−2.055226	−1.163620	−1.991441
83.N	−3.539409	0.590800	−1.752438
84.C	−4.816179	1.113287	−1.665079
85.N	−5.914342	0.353222	−1.555010
86.C	−5.646390	−0.968825	−1.534153
87.C	−4.397177	−1.593058	−1.656680
88.C	−3.233116	−0.786319	−1.806803

89.N	−6.552741	−2.004559	−1.429684
90.C	−5.841106	−3.189281	−1.511738
91.N	−4.543502	−2.978550	−1.654375
92.H	−4.162867	3.119389	−1.665534
93.H	−5.871378	2.813063	−1.507956
94.H	−2.720398	1.230859	−1.806931
95.H	−7.559271	−1.914538	−1.350554
96.H	−6.326874	−4.152125	−1.458865
97.N	2.464672	4.954650	−1.772640
98.O	−1.153862	2.050204	−1.966304
99.N	0.601156	3.538210	−1.759094
100.C	1.122830	4.815966	−1.682976
101.N	0.362662	5.914146	−1.572353
102.C	−0.959013	5.644969	−1.537696
103.C	−1.582708	4.394376	−1.645832
104.C	−0.776185	3.229707	−1.795760
105.N	−1.994918	6.550808	−1.428893
106.C	−3.179285	5.836975	−1.492608
107.N	−2.968207	4.538889	−1.628493
108.H	3.129246	4.164843	−1.690476
109.H	2.822058	5.873913	−1.543202
110.H	1.241726	2.719650	−1.819297
111.H	−1.905534	7.557542	−1.352233
112.H	−4.142473	6.321036	−1.431920
113.N	4.964005	−2.462967	−1.762812
114.O	2.061399	1.154925	−1.992586
115.N	3.547634	−0.599153	−1.763353
116.C	4.825044	−1.120946	−1.680303
117.N	5.922464	−0.360511	−1.569216
118.C	5.652988	0.961019	−1.540639
119.C	4.403214	1.585075	−1.657211
120.C	3.239784	0.778045	−1.810934
121.N	6.558544	1.996695	−1.432184
122.C	5.846079	3.181421	−1.503939
123.N	4.548558	2.970724	−1.645071
124.H	4.173713	−3.127550	−1.682852
125.H	5.881877	−2.819657	−1.527312
126.H	2.729565	−1.239649	−1.823878
127.H	7.564746	1.906608	−1.351733
128.H	6.331055	4.144175	−1.444716

a-G_4-**Na^+**-G_4 (Bond Energy: -19985.65 kcal/mol)			
1.H	5.535942	−5.074409	1.752612
2.C	2.284238	−5.228239	1.723378
3.N	1.077633	−5.824384	1.733679
4.C	2.564366	−3.853816	1.660660
5.C	1.481877	−2.936694	1.586267
6.O	1.531332	−1.681127	1.525842
7.H	−5.533540	5.071777	1.737083
8.N	0.235953	−3.589482	1.579665
9.H	0.593226	2.957106	1.552016
10.H	2.051926	4.822646	1.599216
11.C	4.852709	4.478739	1.626191
12.N	3.646200	3.940865	1.591810
13.H	1.324838	6.428107	1.655010
14.H	−0.589447	−2.957220	1.546897
15.H	−2.049606	−4.822451	1.597436
16.C	0.055376	−4.959405	1.662035
17.N	−5.843854	−3.520080	1.669836
18.N	−1.205615	−5.422055	1.669027
19.C	−4.849915	−4.480334	1.618545
20.N	−3.643504	−3.942187	1.581544
21.C	−3.852407	−2.565354	1.607572
22.C	−2.934569	−1.481934	1.566827
23.O	−1.678115	−1.530771	1.521493
24.N	−3.586958	−0.235928	1.577140

25.C	−4.957937	−0.056925	1.650178
26.N	−5.420465	1.203694	1.677636
27.N	−5.823839	−1.080268	1.692394
28.C	−5.227862	−2.286524	1.660425
29.H	−1.323116	−6.427327	1.661093
30.C	3.855129	2.563894	1.609444
31.C	4.478647	−4.850521	1.729766
32.N	3.941369	−3.644857	1.665440
33.N	3.517343	−5.843662	1.769241
34.N	5.826895	1.078269	1.679270
35.N	5.846763	3.518192	1.667540
36.H	−4.819447	2.049004	1.633021
37.H	4.819889	−2.050215	1.625083
38.H	−6.425409	1.321965	1.658118
39.H	5.076485	5.536180	1.625927
40.H	−5.073625	−5.537724	1.611755
41.H	−2.954689	0.589921	1.556023
42.H	6.427211	−1.325208	1.637179
43.C	2.937069	1.480662	1.567546
44.O	1.680520	1.529698	1.525887
45.H	2.957248	−0.591242	1.554652
46.N	−3.515638	5.842120	1.761585
47.C	5.230778	2.284663	1.655297
48.C	−4.476095	4.848260	1.719718
49.N	3.589466	0.234770	1.572478
50.C	4.960680	0.054873	1.638184
51.N	5.422462	−1.205750	1.657997
52.H	3.687820	−6.842051	1.823099
53.N	−3.938124	3.642727	1.659790
54.C	−2.561216	3.852466	1.661201
55.C	−1.478267	2.935669	1.588896
56.H	6.845912	3.689935	1.702525
57.H	−3.687004	6.840672	1.810823
58.O	−1.527232	1.680224	1.528694
59.N	−0.232488	3.589043	1.584559
60.C	−0.052819	4.959464	1.662636
61.H	−6.843098	−3.691524	1.705125
62.N	1.207824	5.422853	1.667134
63.N	−1.075665	5.824116	1.732054
64.C	−2.282023	5.227265	1.721870
65.N	−2.042156	−5.562504	−1.705064
66.H	−0.226302	6.561392	−1.612901
67.C	0.886982	4.882927	−1.642264
68.C	−3.130963	−4.771934	−1.714188
69.N	−0.278309	5.550876	−1.631688
70.N	2.040417	5.564155	−1.704839
71.N	−5.178181	4.453657	−1.663199
72.C	−4.037007	5.233675	−1.628006
73.N	−2.937585	4.500941	−1.601948
74.C	−3.374985	3.178687	−1.619116
75.C	−2.651769	1.956291	−1.584259
76.O	−1.404894	1.792701	−1.549955
77.N	−3.504590	0.837766	−1.587113
78.C	−4.886803	0.891208	−1.642876
79.N	−5.554461	−0.274098	−1.661093
80.N	−5.568441	2.045595	−1.674954
81.C	−4.777996	3.134327	−1.655021
82.C	1.952935	2.647984	−1.601989
83.O	−1.793278	−1.399404	−1.560060
84.N	−0.836759	−3.498826	−1.582299
85.C	3.129202	4.773516	−1.709444
86.H	−4.080238	6.313656	−1.625991
87.H	−3.020728	−0.082698	−1.574477
88.H	−5.101988	−1.207575	−1.639187
89.H	−6.564896	−0.223197	−1.635689
90.C	−0.888884	−4.881044	−1.640775
91.H	−6.310091	−4.074219	−1.768780
92.H	0.083408	−3.014455	−1.555007
93.H	1.209812	−5.098619	−1.580372

94.H	4.077109	−6.312507	−1.606122
95.H	3.017146	0.084074	−1.583415
96.H	0.223969	−6.559736	−1.610163
97.H	5.099281	1.208628	−1.640112
98.H	6.561362	0.223286	−1.640855
99.C	4.774516	−3.133347	−1.657959
100.N	0.276224	−5.549238	−1.628818
101.N	−4.498524	−2.931556	−1.690394
102.C	−3.176311	−3.369128	−1.673860
103.C	−1.955267	−2.646066	−1.604358
104.N	5.174657	−4.452797	−1.660169
105.C	4.033513	−5.232624	−1.618712
106.N	2.934197	−4.499775	−1.594765
107.C	3.371516	−3.177646	−1.619897
108.C	2.648219	−1.955232	−1.587324
109.O	1.401548	−1.792089	−1.549615
110.N	3.501024	−0.836457	−1.595439
111.N	5.551083	0.275097	−1.672819
112.O	1.790769	1.401192	−1.558324
113.N	0.834420	3.500698	−1.584359
114.C	4.883171	−0.890084	−1.651323
115.H	6.308284	4.075098	−1.750138
116.H	−0.086004	3.017167	−1.558062
117.H	−6.134752	4.789912	−1.687701
118.N	−4.449709	−5.172030	−1.760187
119.C	−5.230409	−4.030830	−1.741381
120.H	−1.211497	5.099356	−1.583449
121.N	5.564729	−2.044568	−1.682411
122.N	4.448071	5.173371	−1.752401
123.C	5.228519	4.032057	−1.727606
124.N	4.496429	2.932987	−1.676647
125.C	3.174232	3.370730	−1.666119
126.H	−4.785758	−6.128309	−1.799992
127.H	4.784059	6.129552	−1.795333
128.H	6.130950	−4.789913	−1.686106
129.Na	0.000274	−0.000281	−0.013944

a-G_4-K^+-G_4 (Bond Energy: -19989.79 kcal/mol)			
1.H	5.550611	−5.138690	1.638162
2.C	2.297511	−5.264146	1.666974
3.N	1.084046	−5.848020	1.680374
4.C	2.590986	−3.890917	1.649030
5.C	1.517952	−2.962287	1.638440
6.O	1.579473	−1.706458	1.634279
7.H	−5.547078	5.144099	1.660811
8.N	0.263549	−3.601345	1.627071
9.H	0.562607	2.970248	1.619901
10.H	2.041968	4.819450	1.625014
11.C	4.907090	4.494761	1.664480
12.N	3.694810	3.968481	1.647367
13.H	1.329910	6.426018	1.616722
14.H	−0.560125	−2.967857	1.627885
15.H	−2.038567	−4.816924	1.636854
16.C	0.069543	−4.971480	1.661251
17.N	−5.892314	−3.522125	1.681249
18.N	−1.197617	−5.420695	1.677963
19.C	−4.905348	−4.491806	1.666932
20.N	−3.692871	−3.965974	1.654103
21.C	−3.892732	−2.587267	1.658014
22.C	−2.964102	−1.514627	1.640940
23.O	−1.708332	−1.576566	1.636250
24.N	−3.602849	−0.260049	1.622879
25.C	−4.973080	−0.065936	1.651728
26.N	−5.422399	1.201226	1.657987
27.N	−5.849800	−1.080360	1.675062
28.C	−5.266001	−2.293942	1.671673
29.H	−1.326666	−6.423138	1.622096

30.C	3.894964	2.589879	1.657832
31.C	4.495477	-4.903981	1.644934
32.N	3.969729	-3.691414	1.635010
33.N	3.525633	-5.890654	1.667779
34.N	5.852262	1.083644	1.693395
35.N	5.894074	3.525434	1.688904
36.H	-4.818633	2.042265	1.620399
37.H	4.822438	-2.038799	1.627754
38.H	-6.424657	1.330020	1.599116
39.H	5.141509	5.549949	1.662249
40.H	-5.139743	-5.546956	1.666496
41.H	-2.969136	0.563665	1.622516
42.H	6.428455	-1.326686	1.628154
43.C	2.966745	1.516763	1.640222
44.O	1.710815	1.578472	1.632106
45.H	2.972587	-0.561481	1.626263
46.N	-3.521795	5.894943	1.681995
47.C	5.268158	2.297081	1.681746
48.C	-4.492101	4.908661	1.662195
49.N	3.606014	0.262441	1.627000
50.C	4.976214	0.068976	1.666382
51.N	5.425873	-1.198224	1.681467
52.H	3.688667	-6.891673	1.682509
53.N	-3.966857	3.695869	1.646434
54.C	-2.587995	3.894928	1.653282
55.C	-1.515620	2.965837	1.636161
56.H	6.894852	3.689939	1.709266
57.H	-3.684691	6.895945	1.701749
58.O	-1.578251	1.709968	1.630774
59.N	-0.260844	3.604108	1.618486
60.C	-0.066360	4.974374	1.653665
61.H	-6.893203	-3.686051	1.696168
62.N	1.201003	5.423186	1.664515
63.N	-1.080241	5.851238	1.679555
64.C	-2.294066	5.267945	1.672128
65.N	-2.051530	-5.589222	-1.670226
66.H	-0.230564	6.559524	-1.611217
67.C	0.901485	4.893412	-1.660115
68.C	-3.149256	-4.809589	-1.665721
69.N	-0.272053	5.550103	-1.671684
70.N	2.049281	5.585883	-1.682018
71.N	-5.221616	4.462770	-1.678940
72.C	-4.085529	5.252368	-1.663066
73.N	-2.978856	4.529941	-1.652322
74.C	-3.408165	3.204582	-1.659183
75.C	-2.673654	1.990528	-1.644407
76.O	-1.425220	1.840546	-1.639440
77.N	-3.514783	0.861643	-1.627833
78.C	-4.898437	0.901447	-1.658227
79.N	-5.555251	-0.271955	-1.668811
80.N	-5.590968	2.049223	-1.679909
81.C	-4.811135	3.146729	-1.673547
82.C	1.990572	2.668565	-1.643201
83.O	-1.843652	-1.423380	-1.636458
84.N	-0.864471	-3.512688	-1.621813
85.C	3.146934	4.806042	-1.673398
86.H	-4.139270	6.331923	-1.661460
87.H	-3.029751	-0.057213	-1.628133
88.H	-5.101155	-1.202040	-1.627546
89.H	-6.564984	-0.230189	-1.611907
90.C	-0.903822	-4.896382	-1.650182
91.H	-6.334689	-4.138400	-1.661914
92.H	0.054053	-3.027243	-1.622913
93.H	1.200322	-5.098865	-1.629080
94.H	4.135173	-6.334509	-1.690884
95.H	3.026184	0.054206	-1.622832
96.H	0.227994	-6.562683	-1.601711
97.H	5.099169	1.199536	-1.614783
98.H	6.562383	0.225863	-1.588680

99.C	4.807657	−3.149937	−1.676711
100.N	0.269546	−5.552943	−1.657000
101.N	−4.533060	−2.977783	−1.650882
102.C	−3.207616	−3.406651	−1.654346
103.C	−1.993753	−2.671610	−1.639651
104.N	5.217401	−4.466050	−1.690939
105.C	4.081252	−5.255077	−1.684731
106.N	2.974641	−4.532381	−1.670433
107.C	3.404603	−3.207281	−1.666447
108.C	2.670334	−1.993393	−1.643698
109.O	1.422073	−1.842923	−1.636063
110.N	3.511728	−0.864396	−1.622914
111.N	5.552920	0.268773	−1.648085
112.O	1.840450	1.420111	−1.638127
113.N	0.861725	3.509893	−1.627689
114.C	4.895519	−0.904290	−1.647928
115.H	6.331809	4.134081	−1.652762
116.H	−0.057288	3.025486	−1.627661
117.H	−6.180777	4.792463	−1.690994
118.N	−4.465154	−5.220516	−1.672710
119.C	−5.255178	−4.084607	−1.661071
120.H	−1.201987	5.095592	−1.630613
121.N	5.587659	−2.052255	−1.672378
122.N	4.462786	5.216527	−1.677681
123.C	5.252319	4.080627	−1.658272
124.N	4.530007	2.973796	−1.647658
125.C	3.204695	3.403047	−1.657570
126.H	−4.794835	−6.179729	−1.686904
127.H	4.792811	6.175677	−1.689403
128.H	6.175766	−4.798239	−1.704235
129.K	−0.000212	0.000169	−0.000750

a-G_4-Rb^+-G_4 (Bond Energy: -19984.00 kcal/mol)			
1.H	5.387756	−5.341051	1.608329
2.C	2.133293	−5.352707	1.687039
3.N	0.898923	−5.891010	1.721328
4.C	2.476542	−3.990831	1.685473
5.C	1.439013	−3.024452	1.726646
6.O	1.548247	−1.772459	1.754904
7.H	−5.391148	5.349309	1.613876
8.N	0.160210	−3.616122	1.731352
9.H	0.636917	2.962614	1.766306
10.H	2.178811	4.755862	1.728637
11.C	5.073127	4.344581	1.623747
12.N	3.843297	3.862749	1.675047
13.H	1.528525	6.380838	1.696052
14.H	−0.641120	−2.956626	1.768175
15.H	−2.183667	−4.751646	1.720231
16.C	−0.082785	−4.978903	1.742738
17.N	−6.024239	−3.336405	1.568250
18.N	−1.366420	−5.383169	1.790582
19.C	−5.072797	−4.340115	1.616872
20.N	−3.843105	−3.858259	1.673683
21.C	−3.995510	−2.473615	1.658176
22.C	−3.031380	−1.434772	1.714574
23.O	−1.780917	−1.542288	1.796057
24.N	−3.621805	−0.157156	1.660978
25.C	−4.983330	0.085937	1.599926
26.N	−5.386404	1.369118	1.582032
27.N	−5.894524	−0.896638	1.562212
28.C	−5.355934	−2.130957	1.590313
29.H	−1.530641	−6.376256	1.681446
30.C	3.995583	2.478180	1.654859
31.C	4.342066	−5.069005	1.634345
32.N	3.860494	−3.838097	1.655600
33.N	3.338329	−6.021677	1.654358

34.N	5.893994	0.900732	1.563711
35.N	6.024603	3.340773	1.572891
36.H	−4.753378	2.188015	1.584213
37.H	4.752310	−2.183346	1.584787
38.H	−6.375137	1.534276	1.442098
39.H	5.345825	5.390364	1.623086
40.H	−5.345316	−5.385964	1.609681
41.H	−2.964595	0.645819	1.702599
42.H	6.375146	−1.530321	1.453102
43.C	3.030642	1.439906	1.704147
44.O	1.780092	1.548041	1.779338
45.H	2.962914	−0.641160	1.696158
46.N	−3.341646	6.029071	1.662100
47.C	5.355979	2.135406	1.590733
48.C	−4.345657	5.076567	1.639444
49.N	3.620720	0.161515	1.653287
50.C	4.982710	−0.081578	1.599818
51.N	5.386021	−1.364946	1.590151
52.H	3.467189	−7.027926	1.656146
53.N	−3.864451	3.845495	1.657032
54.C	−2.480540	3.998017	1.687830
55.C	−1.443418	3.031211	1.723430
56.H	7.030302	3.469880	1.541264
57.H	−3.470184	7.035345	1.666095
58.O	−1.553620	1.779208	1.740157
59.N	−0.164358	3.622136	1.732844
60.C	0.079064	4.984834	1.751619
61.H	−7.029566	−3.465601	1.529764
62.N	1.363023	5.387998	1.805908
63.N	−0.902150	5.897369	1.731075
64.C	−2.136803	5.359584	1.693517
65.N	−1.876712	−5.664350	−1.587519
66.H	−0.433484	6.543282	−1.449784
67.C	0.757167	4.926830	−1.612325
68.C	−3.002975	−4.925855	−1.607274
69.N	−0.439901	5.542879	−1.604346
70.N	1.879011	5.658832	−1.575294
71.N	−5.381853	4.302100	−1.628657
72.C	−4.274675	5.132076	−1.591866
73.N	−3.141488	4.452322	−1.622515
74.C	−3.523781	3.114011	−1.676491
75.C	−2.744687	1.929788	−1.725918
76.O	−1.491918	1.829127	−1.743714
77.N	−3.541252	0.767680	−1.746859
78.C	−4.925400	0.756279	−1.762989
79.N	−5.539177	−0.441502	−1.822683
80.N	−5.660256	1.876261	−1.733072
81.C	−4.923840	3.003106	−1.682780
82.C	1.927119	2.745451	−1.717935
83.O	−1.821313	−1.499672	−1.792139
84.N	−0.765541	−3.548384	−1.671919
85.C	3.005019	4.919968	−1.599757
86.H	−4.368138	6.207831	−1.547817
87.H	−3.025156	−0.132644	−1.785359
88.H	−5.053304	−1.351444	−1.739126
89.H	−6.545317	−0.436892	−1.708413
90.C	−0.754892	−4.931499	−1.622533
91.H	−6.209881	−4.366689	−1.612036
92.H	0.136456	−3.035481	−1.711940
93.H	1.355137	−5.060243	−1.593623
94.H	4.370923	−6.213740	−1.550126
95.H	3.026212	0.126308	−1.777758
96.H	0.436811	−6.549184	−1.475904
97.H	5.054374	1.347003	−1.738667
98.H	6.546308	0.431910	−1.703763
99.C	4.925933	−3.008592	−1.679371
100.N	0.442092	−5.546806	−1.616489
101.N	−4.451478	−3.143399	−1.675899
102.C	−3.112212	−3.526853	−1.666654

103.C	−1.925992	−2.750698	−1.718482
104.N	5.384604	−4.307477	−1.626589
105.C	4.277524	−5.138049	−1.593775
106.N	3.144177	−4.458581	−1.625019
107.C	3.525987	−3.120176	−1.675983
108.C	2.746081	−1.936134	−1.720234
109.O	1.493562	−1.835624	−1.733386
110.N	3.542625	−0.773717	−1.740081
111.N	5.540042	0.436208	−1.817603
112.O	1.822721	1.494763	−1.794230
113.N	0.766648	3.543789	−1.668583
114.C	4.926715	−0.761711	−1.756238
115.H	6.211576	4.359991	−1.609463
116.H	−0.136005	3.031818	−1.709806
117.H	−6.352512	4.596707	−1.625005
118.N	−4.303455	−5.381863	−1.581549
119.C	−5.133100	−4.274579	−1.621811
120.H	−1.352417	5.055462	−1.577493
121.N	5.662120	−1.881279	−1.726106
122.N	4.305572	5.375357	−1.573806
123.C	5.134824	4.268120	−1.619432
124.N	4.452709	3.137392	−1.676378
125.C	3.113546	3.521287	−1.664616
126.H	−4.599276	−6.351575	−1.546034
127.H	4.601645	6.344804	−1.535835
128.H	6.355481	−4.601713	−1.620885
129.Rb	−0.000426	0.001915	−0.002197

a-G_4-**Cs^+**-G_4 (Bond Energy: -19977.50 kcal/mol)

1.H	5.165539	−5.563787	1.543039
2.C	1.913291	−5.444403	1.611912
3.N	0.656466	−5.929602	1.600819
4.C	2.314691	−4.105250	1.748171
5.C	1.320256	−3.105363	1.898621
6.O	1.483983	−1.867316	2.046489
7.H	−5.147708	5.549738	1.484184
8.N	0.016010	−3.638804	1.851704
9.H	0.770706	2.946772	1.975626
10.H	2.388327	4.655592	1.728433
11.C	5.245318	4.115979	1.564673
12.N	4.005434	3.688347	1.726358
13.H	1.805609	6.285593	1.474721
14.H	−0.756754	−2.954824	1.959949
15.H	−2.371459	−4.668767	1.736066
16.C	−0.284932	−4.985569	1.729349
17.N	−6.137177	−3.082456	1.462349
18.N	−1.584398	−5.340428	1.760909
19.C	−5.234078	−4.127686	1.550071
20.N	−3.993360	−3.702181	1.711465
21.C	−4.087524	−2.312591	1.728360
22.C	−3.089253	−1.320351	1.902750
23.O	−1.853995	−1.487185	2.069345
24.N	−3.620585	−0.015031	1.857453
25.C	−4.964639	0.288585	1.713944
26.N	−5.319151	1.588247	1.744757
27.N	−5.907628	−0.651145	1.566614
28.C	−5.424067	−1.908420	1.577410
29.H	−1.788999	−6.305072	1.530075
30.C	4.100678	2.298777	1.734197
31.C	4.132366	−5.251112	1.592745
32.N	3.704072	−4.009269	1.737484
33.N	3.088968	−6.156428	1.509609
34.N	5.921367	0.639662	1.558078
35.N	6.148874	3.072162	1.467108
36.H	−4.646454	2.374790	1.728628
37.H	4.665537	−2.389872	1.729485
38.H	−6.277505	1.792833	1.489274
39.H	5.557869	5.149020	1.511942

40.H	−5.547383	−5.160058	1.490420
41.H	−2.938111	0.756320	1.982279
42.H	6.296757	−1.804398	1.488555
43.C	3.102478	1.304732	1.900487
44.O	1.867314	1.470439	2.068612
45.H	2.951061	−0.772470	1.961897
46.N	−3.070363	6.140241	1.445052
47.C	5.437247	1.896706	1.577920
48.C	−4.114888	5.237489	1.542228
49.N	3.634651	0.000042	1.847172
50.C	4.979047	−0.301487	1.702749
51.N	5.335219	−1.600306	1.732239
52.H	3.174454	−7.163269	1.418536
53.N	−3.688082	3.998387	1.713031
54.C	−2.298562	4.093440	1.726624
55.C	−1.305691	3.097282	1.909797
56.H	7.154190	3.158567	1.360660
57.H	−3.154581	7.145226	1.334964
58.O	−1.471269	1.863501	2.089963
59.N	−0.001038	3.629336	1.856578
60.C	0.301552	4.972531	1.703988
61.H	−7.142478	−3.166733	1.353952
62.N	1.601056	5.327896	1.733045
63.N	−0.638617	5.913918	1.550119
64.C	−1.895552	5.429391	1.564958
65.N	−1.657523	−5.727610	−1.597466
66.H	−0.702850	6.528197	−1.560012
67.C	0.552162	4.968501	−1.731195
68.C	−2.813826	−5.035567	−1.603944
69.N	−0.666992	5.541138	−1.784460
70.N	1.640861	5.740018	−1.610569
71.N	−5.548778	4.091072	−1.524381
72.C	−4.476377	4.964201	−1.588924
73.N	−3.322981	4.329379	−1.705743
74.C	−3.655244	2.976840	−1.717037
75.C	−2.837834	1.825443	−1.849928
76.O	−1.587887	1.774673	−1.976043
77.N	−3.588050	0.631484	−1.817056
78.C	−4.968281	0.565578	−1.723881
79.N	−5.541078	−0.653560	−1.770505
80.N	−5.739629	1.655284	−1.612284
81.C	−5.045862	2.810555	−1.611996
82.C	1.813944	2.839263	−1.852510
83.O	−1.781759	−1.578030	−1.979108
84.N	−0.636338	−3.575798	−1.813490
85.C	2.796823	5.047019	−1.604443
86.H	−4.609165	6.035860	−1.548445
87.H	−3.043606	−0.246615	−1.912228
88.H	−5.015371	−1.544074	−1.733285
89.H	−6.529817	−0.688829	−1.554258
90.C	−0.568368	−4.955123	−1.709667
91.H	−6.039848	−4.602081	−1.548052
92.H	0.241527	−3.031286	−1.910961
93.H	1.540874	−4.996850	−1.702334
94.H	4.597599	−6.020241	−1.491065
95.H	3.028595	0.257242	−1.922849
96.H	0.688381	−6.512593	−1.519270
97.H	4.998552	1.557128	−1.739000
98.H	6.513236	0.704026	−1.562960
99.C	5.032891	−2.795896	−1.595740
100.N	0.652210	−5.525440	−1.742621
101.N	−4.334485	−3.314807	−1.708483
102.C	−2.981581	−3.645823	−1.716136
103.C	−1.830940	−2.827792	−1.850032
104.N	5.536385	−4.075084	−1.492826
105.C	4.464560	−4.949482	−1.548378
106.N	3.311109	−4.316742	−1.676009
107.C	3.642932	−2.964274	−1.703454
108.C	2.824816	−1.814579	−1.846862

109.O	1.574917	−1.766409	−1.971539
110.N	3.574048	−0.619682	−1.822608
111.N	5.526062	0.667723	−1.786979
112.O	1.765980	1.589022	−1.975069
113.N	0.619156	3.588467	−1.827269
114.C	4.953839	−0.551898	−1.729073
115.H	6.021581	4.610174	−1.518493
116.H	−0.258548	3.043391	−1.923503
117.H	−6.528494	4.347449	−1.462490
118.N	−4.094096	−5.539652	−1.517878
119.C	−4.968298	−4.468449	−1.588263
120.H	−1.556426	5.013513	−1.741598
121.N	5.725870	−1.639933	−1.606742
122.N	4.076698	5.549641	−1.506036
123.C	4.950355	4.477691	−1.568203
124.N	4.316636	3.324630	−1.694234
125.C	2.964265	3.657116	−1.714623
126.H	−4.350362	−6.518799	−1.447129
127.H	4.332897	6.528612	−1.434156
128.H	6.515076	−4.330823	−1.414528
129.Cs	−0.004213	0.003523	0.040537

Table S5. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of GQ-M^+ at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory

GQ-**Li**$^+$ (Bond Energy: -38293.9 kcal/mol)			
1.C	6.427317	−0.914212	1.460157
2.N	5.242254	−0.336159	1.508851
3.C	4.308527	−1.370768	1.474840
4.C	2.887014	−1.370625	1.459025
5.O	2.113161	−0.371672	1.482642
6.N	2.359384	−2.670832	1.406891
7.C	3.109628	−3.839734	1.387217
8.N	2.462884	−5.015937	1.378087
9.N	4.447588	−3.835604	1.396939
10.C	4.972933	−2.604769	1.427053
11.H	10.549865	−1.969333	3.057499
12.H	11.595965	−2.501811	1.721251
13.H	10.104002	−4.285889	2.402877
14.H	10.302270	−3.739989	−0.293591
15.H	8.417939	−2.151005	−0.233180
16.H	7.659935	−3.620113	−0.892367
17.H	6.845810	−4.259518	1.335667
18.H	7.384897	−0.412854	1.469092
19.H	1.323497	−2.695424	1.371942
20.H	1.429831	−5.047436	1.283516
21.H	3.016214	−5.826936	1.108424
22.P	8.562970	−6.218989	−0.769534
23.O	9.003636	−7.724514	−0.444112
24.O	8.834436	−5.680024	−2.129827
25.O	6.986197	−6.270434	−0.505269
26.C	6.358054	−6.971895	0.636651
27.C	−2.970485	−1.452339	−1.666071
28.C	5.287864	−7.951984	0.153636
29.O	3.999059	−7.300545	−0.088123
30.C	5.607807	−8.690909	−1.164526
31.O	5.077647	−10.037826	−1.173896
32.C	4.966744	−7.784690	−2.233577
33.C	3.763756	−7.140021	−1.521021
34.C	−4.204563	1.484438	1.733790
35.N	3.553504	−5.728855	−1.827290
36.C	−2.785071	1.492131	1.647814
37.H	−4.828438	2.100441	−1.567119
38.N	−3.601668	−0.192841	−1.579053
39.N	−4.952936	−2.344075	2.082448
40.H	−6.420996	1.382044	−1.332978
41.C	−4.961779	−0.001164	−1.420541
42.H	−7.341685	−5.547136	−1.627494
43.O	−1.735384	−1.518386	−1.859355
44.H	−8.637868	−4.422411	−2.077567
45.C	8.172545	−3.196784	−0.027699
46.N	−2.282315	−6.200290	1.528310
47.H	−5.098691	−5.475740	−1.111444
48.H	−7.650505	−7.039802	2.056345
49.H	−9.102478	−6.401939	−0.240231
50.H	−7.551699	3.817936	−0.443789
51.C	4.509534	−4.714160	−1.868573
52.N	3.965018	−3.515631	−1.937692
53.O	−0.358539	−1.988051	1.408088
54.C	−3.791567	−2.989781	1.872778
55.C	−1.999356	−10.405130	1.865090
56.N	−2.636156	−2.237550	1.712922
57.C	7.364077	−3.301324	1.268134
58.C	−5.240976	−2.223889	−1.267450
59.O	−2.006947	0.497519	1.617690
60.H	−9.794462	0.928948	1.998960

61.N	−5.123226	0.440238	1.791051
62.N	−3.788997	−4.327128	1.850674
63.C	−2.574196	−4.851155	1.646074
64.N	−5.427736	1.260587	−1.475273
65.O	1.486046	10.600671	1.380329
66.C	2.562499	10.753100	2.336307
67.C	3.617354	9.653827	2.243048
68.O	3.014553	8.361978	2.612052
69.C	4.225503	9.447971	0.838325
70.O	5.668122	9.179081	1.064621
71.C	3.489942	8.216795	0.314831
72.C	3.363745	7.392211	1.596889
73.N	2.377065	6.332824	1.566841
74.C	0.992698	6.425758	1.463171
75.N	0.419388	5.239068	1.431657
76.C	1.456519	4.311761	1.497354
77.C	1.457629	2.889744	1.478924
78.O	0.460170	2.119048	1.405671
79.N	2.754781	2.362390	1.554374
80.C	3.918541	3.112443	1.656803
81.N	5.088498	2.458359	1.756558
82.N	3.913952	4.451384	1.683143
83.C	2.686205	4.979569	1.591102
84.H	2.168215	10.783070	3.359155
85.H	3.039931	11.713026	2.117436
86.H	4.418224	9.881574	2.955726
87.H	4.144164	10.324641	0.196006
88.H	2.498218	8.524769	−0.031982
89.H	4.002151	7.695485	−0.494424
90.H	4.309068	6.902820	1.845419
91.H	0.478314	7.374432	1.433049
92.H	2.786926	1.326143	1.526437
93.H	5.124250	1.430287	1.617276
94.H	5.919295	3.003692	1.528802
95.P	6.590767	8.518227	−0.075393
96.O	8.068561	8.858697	0.441666
97.O	6.227339	8.885140	−1.470893
98.O	6.527391	6.932605	0.113185
99.C	7.100399	6.214816	1.272596
100.C	8.087202	5.144317	0.805500
101.O	7.419105	3.893866	0.443032
102.C	8.922721	5.512374	−0.440051
103.O	10.245716	4.927233	−0.396808
104.C	8.063677	4.975730	−1.603478
105.C	7.328969	3.760334	−1.009489
106.N	5.931507	3.619641	−1.407909
107.C	4.935894	4.596750	−1.472289
108.N	3.736294	4.079923	−1.658224
109.C	3.929780	2.697162	−1.699123
110.C	2.993418	1.629527	−1.796251
111.O	1.747881	1.699494	−1.896601
112.N	3.625739	0.368057	−1.756757
113.C	4.992955	0.172316	−1.689693
114.N	5.452594	−1.088829	−1.778044
115.N	5.868372	1.179180	−1.557962
116.C	5.287798	2.393101	−1.552218
117.H	6.262200	5.748578	1.794686
118.H	7.608241	6.927026	1.924969
119.H	8.735291	4.909877	1.655630
120.H	9.092033	6.586181	−0.517285
121.H	7.354814	5.741410	−1.921790
122.H	8.678389	4.693477	−2.460858
123.H	7.798629	2.811325	−1.272494
124.H	5.163760	5.644737	−1.360622
125.H	2.978717	−0.445689	−1.800710
126.H	4.846685	−1.928309	−1.835910
127.H	6.452494	−1.210824	−1.695448
128.H	−5.651743	7.278794	−2.140115
129.H	−4.625052	8.616972	−2.682458

130.O	-1.086528	-9.803723	0.912929
131.H	-2.751541	7.808929	-1.427409
132.H	-5.536120	5.129804	-1.490633
133.H	0.587254	3.004209	-1.758391
134.H	2.053648	4.888476	-1.741529
135.H	1.314247	6.475741	-1.713515
136.H	-6.820281	4.339741	1.877616
137.H	-7.257920	0.482790	1.849290
138.H	4.112393	-9.997862	-1.039368
139.H	-1.236439	2.828209	1.501186
140.C	-4.483725	4.912131	-1.575593
141.N	-3.950241	3.712502	-1.699092
142.C	-2.570020	3.919799	-1.727067
143.C	-1.494227	2.988477	-1.758558
144.O	-1.557879	1.739212	-1.794239
145.N	1.204163	5.475007	-1.812321
146.N	-1.072721	5.877321	-1.637662
147.C	-2.282612	5.285959	-1.634537
148.H	-5.736832	6.309914	1.653276
149.H	-1.352444	5.165197	1.474039
150.H	10.159325	3.958982	-0.316437
151.H	-2.937944	5.952439	1.362929
152.P	-8.436450	6.415421	-0.322762
153.O	-8.850524	7.927585	0.007344
154.O	-8.743598	5.879602	-1.676407
155.O	-6.856190	6.441992	-0.087667
156.C	-6.203424	7.102059	1.063523
157.N	-0.239555	3.636718	-1.730882
158.H	-8.055340	-9.914010	0.471535
159.C	-5.142529	8.093013	0.585400
160.O	-3.871168	7.439920	0.269239
161.C	-5.503485	8.885009	-0.690404
162.C	-3.290237	-7.243008	1.514334
163.N	-0.328363	-5.115926	1.314824
164.C	-1.349254	-4.184827	1.499259
165.H	-7.717767	-2.659856	-0.736049
166.C	-1.348654	-2.763352	1.528862
167.H	-1.539460	-10.447820	2.860418
168.H	-2.269788	-11.425265	1.556146
169.H	-3.947247	-10.093094	2.665775
170.H	-2.408456	-8.192893	-0.224242
171.H	-3.994547	-7.464461	-0.560272
172.H	-4.223942	-6.737617	1.767726
173.H	-0.421135	-7.258551	1.212466
174.O	-10.502398	1.468210	1.604524
175.H	-8.577109	-4.886634	2.014120
176.H	-2.961359	0.623350	-1.660750
177.H	-2.669133	-1.201260	1.706239
178.H	-5.002755	-1.317593	1.939214
179.H	-5.787133	-2.899027	1.892297
180.P	-6.483041	-8.476924	-0.016510
181.O	-7.897019	-8.954158	0.565654
182.O	-6.197686	-8.712908	-1.458200
183.N	-2.268661	2.794859	1.588181
184.O	-6.500523	-6.908788	0.293128
185.C	-7.070985	-6.293641	1.510115
186.C	-7.967738	-5.117281	1.134210
187.O	-7.196131	-3.915370	0.828410
188.C	-8.860676	-5.344388	-0.095129
189.O	-10.074548	-4.578947	0.121000
190.C	-8.018001	-4.777375	-1.250797
191.O	-5.441121	-9.170646	0.995130
192.C	-10.675476	2.634222	2.445386
193.N	-5.824211	-1.010765	-1.235122
194.C	-9.571524	3.673286	2.271015
195.O	-8.289136	3.104674	2.720205
196.C	-3.402165	-7.995604	0.184697
197.C	-7.232042	-3.627618	-0.600657
198.N	-5.868992	-3.454216	-1.092037

199.C	−4.877981	−4.426576	−1.229492
200.C	−9.340510	4.141438	0.816638
201.H	−3.914903	−10.132268	−0.081429
202.O	−9.093961	5.602766	0.899785
203.C	−8.090233	3.374609	0.394499
204.C	−7.297704	3.371646	1.703332
205.N	−3.693775	−3.906004	−1.488842
206.C	−3.025980	3.958802	1.623571
207.N	−2.380426	5.135511	1.607690
208.N	−4.363534	3.947869	1.693076
209.C	−4.881644	2.713184	1.733212
210.H	−10.729715	2.343058	3.501174
211.C	−3.893862	−2.523188	−1.504620
212.C	−3.277755	−9.581118	1.967743
213.O	−2.995186	−8.246467	2.513111
214.N	−6.231691	2.393868	1.779539
215.C	−4.004504	−9.319505	0.639397
216.H	−11.628517	3.087775	2.157298
217.O	10.119329	−1.067815	1.269181
218.H	−9.808185	4.541071	2.897409
219.C	10.567581	−2.238418	1.997199
220.C	9.672809	−3.467898	1.814943
221.O	8.328579	−3.189969	2.338522
222.H	−10.202225	3.983009	0.168732
223.C	9.452402	−3.927225	0.363985
224.H	−8.381190	2.351774	0.133245
225.H	−10.625457	−4.677959	−0.676886
226.O	9.243312	−5.397205	0.435800
227.C	2.586657	−3.730828	−1.922508
228.C	1.507510	−2.803867	−1.881800
229.O	1.566529	−1.554098	−1.880879
230.N	0.257604	−3.458184	−1.822883
231.C	0.081199	−4.827552	−1.840007
232.N	−1.182988	−5.298170	−1.902280
233.N	1.101873	−5.697229	−1.829762
234.C	2.309638	−5.100789	−1.858325
235.H	5.901288	−6.203324	1.264034
236.H	7.124646	−7.512310	1.194872
237.H	5.123460	−8.665505	0.967328
238.H	6.680636	−8.808717	−1.317279
239.H	5.683828	−7.024907	−2.548254
240.H	4.657008	−8.353498	−3.112756
241.H	2.818125	−7.633293	−1.751805
242.H	5.565706	−4.927041	−1.824988
243.H	−0.571466	−2.828158	−1.797310
244.H	−2.023211	−4.716995	−1.735933
245.H	−1.284219	−6.300727	−1.809326
246.O	−4.960760	10.226380	−0.667673
247.C	−4.913498	8.014775	−1.818402
248.C	−3.696368	7.323818	−1.177632
249.C	−0.056876	5.005337	−1.716115
250.H	−6.955940	7.625882	1.656103
251.H	−4.940526	8.771482	1.420152
252.H	−3.992141	10.172583	−0.566856
253.C	−6.314040	1.004920	1.803190
254.Li	0.051701	0.063595	1.305076
255.H	8.274764	9.813795	0.447444
256.N	−3.519593	5.920658	−1.539276
257.H	−6.233950	−5.942754	2.117379
258.H	−6.579832	9.017987	−0.797483
259.H	−0.242388	−10.283730	0.974778
260.H	0.914844	9.879415	1.698462
261.H	−9.814077	8.087941	−0.028605
262.N	6.324647	−2.301599	1.414148
263.C	−0.909633	−6.300398	1.325402
264.H	10.543705	−1.070647	0.393338
265.H	9.969918	−7.867708	−0.475489

GQ-**Na**$^{+}$ (Bond Energy: -38284.8 kcal/mol)

1.C	6.534423	−0.923184	1.402122
2.N	5.355767	−0.330813	1.435769
3.C	4.413806	−1.359202	1.440382
4.C	2.993534	−1.339676	1.395775
5.O	2.235841	−0.335648	1.339369
6.N	2.445791	−2.636606	1.401032
7.C	3.179742	−3.812981	1.419785
8.N	2.517572	−4.982834	1.439991
9.N	4.518734	−3.826708	1.431620
10.C	5.061846	−2.601166	1.429559
11.H	10.655641	−2.069610	3.047770
12.H	11.695369	−2.623932	1.715463
13.H	10.159024	−4.374967	2.378075
14.H	10.371161	−3.806177	−0.314874
15.H	8.516683	−2.183992	−0.242088
16.H	7.730734	−3.633180	−0.911173
17.H	6.910898	−4.276095	1.316242
18.H	7.497436	−0.432457	1.395801
19.H	1.407240	−2.658717	1.366722
20.H	1.484329	−5.028548	1.362671
21.H	3.062786	−5.805321	1.190303
22.P	8.567383	−6.246057	−0.805831
23.O	8.988513	−7.762828	−0.506633
24.O	8.823953	−5.697933	−2.165391
25.O	6.994989	−6.272200	−0.512437
26.C	6.380375	−6.977316	0.635000
27.C	−2.939196	−1.381662	−1.550808
28.C	5.297347	−7.948100	0.162916
29.O	4.010340	−7.284993	−0.055901
30.C	5.593097	−8.681489	−1.164031
31.O	5.054903	−10.025149	−1.173439
32.C	4.941620	−7.764735	−2.217579
33.C	3.748981	−7.125795	−1.483656
34.C	−4.291686	1.472200	1.679603
35.N	3.525996	−5.714757	−1.784539
36.C	−2.874090	1.461217	1.574059
37.H	−4.835406	2.131339	−1.588049
38.N	−3.594415	−0.136241	−1.529145
39.N	−4.911010	−2.365621	1.947761
40.H	−6.444090	1.401944	−1.495058
41.C	−4.966571	0.035278	−1.483556
42.H	−7.256107	−5.572825	−1.732392
43.O	−1.683052	−1.425803	−1.570735
44.H	−8.565433	−4.492629	−2.248867
45.C	8.252063	−3.226358	−0.043690
46.N	−2.272404	−6.275026	1.626611
47.H	−5.035189	−5.438947	−1.174943
48.H	−7.611453	−6.946003	2.004424
49.H	−9.030798	−6.421044	−0.358535
50.H	−7.620198	3.825586	−0.474189
51.C	4.471667	−4.691105	−1.820460
52.N	3.915980	−3.497113	−1.873319
53.O	−0.301299	−2.100369	1.348451
54.C	−3.750313	−3.032556	1.808047
55.C	−2.100040	−10.503367	1.932453
56.N	−2.582051	−2.302381	1.654834
57.C	7.442752	−3.325117	1.251810
58.C	−5.221522	−2.191631	−1.372996
59.O	−2.116304	0.462655	1.462420
60.H	−9.884044	0.984446	2.012858
61.N	−5.220259	0.434838	1.686001
62.N	−3.766019	−4.370854	1.838246
63.C	−2.551294	−4.919036	1.693362
64.N	−5.442111	1.289853	−1.570161
65.O	1.569551	10.681328	1.726348
66.C	2.714669	10.794806	2.604736
67.C	3.735956	9.676984	2.413382

68.O	3.121887	8.389944	2.780089
69.C	4.252263	9.501417	0.967553
70.O	5.702487	9.205637	1.093767
71.C	3.466418	8.297262	0.456862
72.C	3.396506	7.441207	1.722416
73.N	2.393251	6.398460	1.713541
74.C	1.007657	6.511812	1.620420
75.N	0.417982	5.333937	1.561855
76.C	1.446457	4.394347	1.598987
77.C	1.426960	2.976215	1.505950
78.O	0.424016	2.228184	1.372390
79.N	2.719314	2.424023	1.563546
80.C	3.892653	3.153275	1.677008
81.N	5.058290	2.481812	1.727347
82.N	3.907786	4.491066	1.754390
83.C	2.685241	5.040555	1.700491
84.H	2.394332	10.809325	3.653356
85.H	3.193877	11.750144	2.371186
86.H	4.585114	9.863997	3.080979
87.H	4.145202	10.397543	0.356933
88.H	2.462346	8.629425	0.174500
89.H	3.923138	7.788492	-0.392947
90.H	4.345055	6.930831	1.907900
91.H	0.506939	7.468409	1.618391
92.H	2.748152	1.388234	1.482812
93.H	5.103882	1.459338	1.561607
94.H	5.890941	3.028388	1.512432
95.P	6.540588	8.557584	-0.116717
96.O	8.052687	8.869411	0.313471
97.O	6.096441	8.957588	-1.479265
98.O	6.472043	6.967283	0.043990
99.C	7.074602	6.239180	1.184216
100.C	8.060510	5.177444	0.693164
101.O	7.397172	3.915303	0.359919
102.C	8.856908	5.544827	-0.577534
103.O	10.186446	4.973260	-0.567295
104.C	7.971389	4.988603	-1.710862
105.C	7.280166	3.762471	-1.088473
106.N	5.875800	3.590382	-1.450193
107.C	4.859903	4.546541	-1.438809
108.N	3.662988	4.008188	-1.565395
109.C	3.878309	2.630936	-1.648545
110.C	2.962169	1.543814	-1.666027
111.O	1.706371	1.587838	-1.630181
112.N	3.618503	0.299533	-1.702260
113.C	4.991752	0.129442	-1.723423
114.N	5.464560	-1.121716	-1.854766
115.N	5.852526	1.152875	-1.634660
116.C	5.250302	2.353538	-1.584317
117.H	6.249161	5.763601	1.718293
118.H	7.589555	6.948522	1.834284
119.H	8.735552	4.957030	1.525904
120.H	9.012331	6.619389	-0.668200
121.H	7.236527	5.739511	-2.005667
122.H	8.561690	4.715753	-2.588154
123.H	7.764059	2.821682	-1.354893
124.H	5.071721	5.597486	-1.318311
125.H	2.981771	-0.521955	-1.713098
126.H	4.856382	-1.963285	-1.855549
127.H	6.468355	-1.233188	-1.810053
128.H	-5.622933	7.237661	-2.134312
129.H	-4.590652	8.570613	-2.680493
130.O	-1.149484	-9.924769	1.003561
131.H	-2.736961	7.791191	-1.376486
132.H	-5.497423	5.086032	-1.439328
133.H	0.642226	3.019246	-1.602020
134.H	2.084672	4.905544	-1.631616
135.H	1.340968	6.504747	-1.620637
136.H	-6.872806	4.354095	1.845046

137.H	−7.355299	0.501766	1.733238
138.H	4.092141	−9.980752	−1.023674
139.H	−1.299792	2.790767	1.502882
140.C	−4.442053	4.878138	−1.516648
141.N	−3.895439	3.682573	−1.617618
142.C	−2.516743	3.902246	−1.645671
143.C	−1.427703	2.989095	−1.620134
144.O	−1.473348	1.732920	−1.587003
145.N	1.237436	5.501153	−1.692780
146.N	−1.046153	5.880940	−1.566454
147.C	−2.246410	5.275126	−1.571839
148.H	−5.781801	6.305752	1.649414
149.H	−1.384979	5.143727	1.566152
150.H	10.112969	4.006867	−0.457424
151.H	−2.962429	5.929566	1.462207
152.P	−8.456666	6.430820	−0.361649
153.O	−8.853243	7.951241	−0.047266
154.O	−8.755906	5.890736	−1.715404
155.O	−6.878449	6.436428	−0.106616
156.C	−6.236878	7.098018	1.051005
157.N	−0.184966	3.649938	−1.607347
158.H	−8.118512	−9.808938	0.393309
159.C	−5.164760	8.082618	0.584558
160.O	−3.889691	7.422260	0.299078
161.C	−5.499275	8.863839	−0.705133
162.C	−3.296697	−7.300807	1.582607
163.N	−0.298405	−5.220622	1.425637
164.C	−1.314808	−4.274843	1.556707
165.H	−7.716785	−2.667253	−0.944264
166.C	−1.296393	−2.854572	1.510972
167.H	−1.663016	−10.567012	2.937022
168.H	−2.395280	−11.512612	1.610798
169.H	−4.054931	−10.136220	2.692872
170.H	−2.393449	−8.256607	−0.140585
171.H	−3.951294	−7.482796	−0.511581
172.H	−4.228036	−6.783485	1.820438
173.H	−0.417578	−7.364791	1.384726
174.O	−10.590656	1.524113	1.616296
175.H	−8.590145	−4.823435	1.856988
176.H	−2.958378	0.685156	−1.553185
177.H	−2.612685	−1.265183	1.602890
178.H	−4.965568	−1.341323	1.797646
179.H	−5.747907	−2.915003	1.754603
180.P	−6.478101	−8.437158	−0.046101
181.O	−7.918376	−8.859720	0.514292
182.O	−6.173506	−8.697267	−1.479896
183.N	−2.334648	2.760153	1.585171
184.O	−6.443498	−6.866597	0.249021
185.C	−7.041586	−6.212447	1.431766
186.C	−7.956493	−5.069558	0.998719
187.O	−7.202577	−3.861372	0.671435
188.C	−8.815438	−5.354827	−0.242591
189.O	−10.051023	−4.611399	−0.080209
190.C	−7.957618	−4.806425	−1.397133
191.O	−5.481750	−9.158628	0.992541
192.C	−10.746075	2.703262	2.442133
193.N	−5.823437	−0.989098	−1.371524
194.C	−9.628356	3.724408	2.251406
195.O	−8.352465	3.140381	2.697927
196.C	−3.392777	−8.037392	0.242725
197.C	−7.213324	−3.618940	−0.767251
198.N	−5.840353	−3.430454	−1.227101
199.C	−4.826537	−4.386560	−1.288149
200.C	−9.399721	4.177315	0.791412
201.H	−3.958360	−10.157151	−0.054384
202.O	−9.140660	5.637638	0.859161
203.C	−8.159381	3.394784	0.370270
204.C	−7.360918	3.390703	1.675374
205.N	−3.637007	−3.848257	−1.471019

206.C	−3.074916	3.930492	1.663579
207.N	−2.413337	5.100737	1.682629
208.N	−4.413553	3.936800	1.732124
209.C	−4.951064	2.707945	1.726253
210.H	−10.801453	2.426706	3.501819
211.C	−3.854914	−2.468784	−1.515756
212.C	−3.354037	−9.640714	2.013826
213.O	−3.039187	−8.319672	2.575092
214.N	−6.306028	2.402277	1.748568
215.C	−4.041949	−9.347779	0.670727
216.H	−11.693768	3.165744	2.150603
217.O	10.257334	−1.152730	1.260346
218.H	−9.848981	4.601266	2.871024
219.C	10.672387	−2.336198	1.986959
220.C	9.748112	−3.542316	1.796050
221.O	8.411058	−3.234746	2.321678
222.H	−10.265974	4.021182	0.148880
223.C	9.517885	−3.984133	0.340741
224.H	−8.461503	2.373406	0.116240
225.H	−10.594864	−4.777196	−0.871956
226.O	9.283614	−5.451239	0.396627
227.C	2.538675	−3.723258	−1.855537
228.C	1.448936	−2.815108	−1.763255
229.O	1.493035	−1.560044	−1.702996
230.N	0.210258	−3.480568	−1.711195
231.C	0.046643	−4.853263	−1.748709
232.N	−1.210257	−5.332459	−1.789714
233.N	1.078726	−5.709042	−1.766200
234.C	2.276786	−5.098821	−1.803728
235.H	5.938114	−6.209647	1.273585
236.H	7.152399	−7.524696	1.178540
237.H	5.140149	−8.665023	0.975102
238.H	6.662725	−8.805035	−1.333166
239.H	5.656121	−7.002311	−2.532101
240.H	4.620558	−8.324290	−3.098723
241.H	2.801469	−7.622261	−1.699374
242.H	5.530461	−4.894368	−1.785790
243.H	−0.617415	−2.853448	−1.646811
244.H	−2.052527	−4.741919	−1.657847
245.H	−1.309031	−6.337604	−1.735270
246.O	−4.951960	10.203360	−0.686087
247.C	−4.891040	7.980098	−1.812438
248.C	−3.683396	7.301493	−1.142131
249.C	−0.017310	5.022744	−1.614988
250.H	−6.994702	7.626811	1.632129
251.H	−4.976089	8.767293	1.417314
252.H	−3.985764	10.147269	−0.565761
253.C	−6.404375	1.012828	1.714473
254.Na	0.037193	0.072955	0.102606
255.H	8.266512	9.822392	0.343235
256.N	−3.489724	5.896736	−1.491338
257.H	−6.215500	−5.820445	2.028864
258.H	−6.572797	8.999436	−0.833677
259.H	−0.321984	−10.430910	1.080116
260.H	1.020628	9.950161	2.061148
261.H	−9.814391	8.123416	−0.092795
262.N	6.417540	−2.312214	1.400969
263.C	−0.895259	−6.397427	1.457920
264.H	10.680048	−1.167334	0.383834
265.H	9.951267	−7.921709	−0.563715

GQ-$\mathbf{K}^{+}$ (Bond Energy: -38288.0 kcal/mol)

1.C	6.558083	−0.973277	1.538440
2.N	5.382569	−0.379432	1.627034
3.C	4.441017	−1.408658	1.621143
4.C	3.022147	−1.383957	1.631169
5.O	2.267896	−0.376847	1.655291

6.N	2.466774	−2.678995	1.588969
7.C	3.195429	−3.857327	1.540039
8.N	2.527363	−5.025136	1.531432
9.N	4.534654	−3.875328	1.516504
10.C	5.083267	−2.651144	1.546678
11.H	10.725066	−2.079038	2.965401
12.H	11.706344	−2.597518	1.575518
13.H	10.238356	−4.385058	2.311132
14.H	10.326670	−3.822222	−0.386178
15.H	8.458710	−2.218520	−0.236033
16.H	7.662834	−3.676767	−0.874468
17.H	6.931913	−4.324359	1.379552
18.H	7.523245	−0.486821	1.518900
19.H	1.427640	−2.707316	1.592075
20.H	1.494848	−5.080686	1.482979
21.H	3.068065	−5.845340	1.263817
22.P	8.533390	−6.280014	−0.802876
23.O	8.974804	−7.792638	−0.512071
24.O	8.741788	−5.733581	−2.171126
25.O	6.971541	−6.315685	−0.459618
26.C	6.392560	−7.018991	0.706685
27.C	−3.015732	−1.477312	−1.511022
28.C	5.301696	−7.996302	0.269178
29.O	4.012081	−7.333165	0.062696
30.C	5.573626	−8.751613	−1.050648
31.O	5.040325	−10.096789	−1.027279
32.C	4.899693	−7.855103	−2.107258
33.C	3.721227	−7.203708	−1.361592
34.C	−4.388954	1.382847	1.864514
35.N	3.491813	−5.798622	−1.686000
36.C	−2.970657	1.364430	1.799880
37.H	−4.886635	2.054991	−1.459197
38.N	−3.658147	−0.225494	−1.463741
39.N	−4.918689	−2.483544	2.118243
40.H	−6.488124	1.337419	−1.272911
41.C	−5.025357	−0.042759	−1.345467
42.H	−7.354967	−5.622436	−1.545783
43.O	−1.762687	−1.530403	−1.610762
44.H	−8.665210	−4.523192	−2.016396
45.C	8.214160	−3.264014	−0.028678
46.N	−2.309140	−6.411497	1.716985
47.H	−5.115887	−5.515863	−1.007830
48.H	−7.638838	−7.056683	2.171567
49.H	−9.106669	−6.479100	−0.148812
50.H	−7.686134	3.764146	−0.354776
51.C	4.437822	−4.775967	−1.750846
52.N	3.883590	−3.583177	−1.833683
53.O	−0.297363	−2.253702	1.612860
54.C	−3.763041	−3.160139	1.969479
55.C	−2.158152	−10.647437	1.938616
56.N	−2.586155	−2.438184	1.850516
57.C	7.458237	−3.371625	1.298427
58.C	−5.289794	−2.268334	−1.209296
59.O	−2.213571	0.361555	1.749662
60.H	−9.976495	0.908553	2.067863
61.N	−5.318027	0.345484	1.883414
62.N	−3.791079	−4.498692	1.963266
63.C	−2.579245	−5.055984	1.816392
64.N	−5.493138	1.216713	−1.404739
65.O	1.574342	10.688118	1.506368
66.C	2.661136	10.835879	2.451908
67.C	3.685873	9.707437	2.376186
68.O	3.052978	8.441844	2.784964
69.C	4.268380	9.451856	0.968819
70.O	5.707500	9.151331	1.179226
71.C	3.495722	8.226570	0.486898
72.C	3.367397	7.438628	1.792132
73.N	2.358209	6.399904	1.800903
74.C	0.970570	6.519162	1.736994

75.N	0.371660	5.343898	1.719567
76.C	1.398628	4.402009	1.753890
77.C	1.367398	2.983255	1.714567
78.O	0.357538	2.237779	1.640719
79.N	2.657682	2.420991	1.750149
80.C	3.838351	3.143072	1.824714
81.N	4.998634	2.461399	1.881057
82.N	3.864214	4.482881	1.861398
83.C	2.643867	5.041084	1.812939
84.H	2.274998	10.900432	3.476203
85.H	3.161777	11.777099	2.205877
86.H	4.501606	9.931194	3.073208
87.H	4.198505	10.314806	0.307247
88.H	2.506891	8.549498	0.145515
89.H	3.984558	7.672118	-0.314984
90.H	4.305972	6.935913	2.040795
91.H	0.477315	7.479340	1.728595
92.H	2.686779	1.383215	1.716731
93.H	5.045007	1.436244	1.743893
94.H	5.836831	2.994455	1.651803
95.P	6.594808	8.465620	0.025750
96.O	8.089207	8.767803	0.517961
97.O	6.217507	8.839016	-1.364370
98.O	6.495080	6.881060	0.217394
99.C	7.070129	6.154821	1.371309
100.C	8.045111	5.075850	0.896720
101.O	7.362780	3.827881	0.549560
102.C	8.867885	5.431403	-0.360995
103.O	10.187593	4.838465	-0.330837
104.C	7.990877	4.892667	-1.509734
105.C	7.268549	3.678076	-0.900391
106.N	5.868400	3.525729	-1.286872
107.C	4.861699	4.492955	-1.302390
108.N	3.662852	3.969299	-1.468825
109.C	3.868727	2.589766	-1.550063
110.C	2.946104	1.513799	-1.621541
111.O	1.689381	1.570078	-1.645263
112.N	3.587881	0.260855	-1.638063
113.C	4.959819	0.074690	-1.601734
114.N	5.422221	-1.182428	-1.704233
115.N	5.826017	1.089579	-1.478746
116.C	5.235310	2.296364	-1.443848
117.H	6.229795	5.696201	1.896985
118.H	7.588323	6.860971	2.022116
119.H	8.702559	4.841343	1.739602
120.H	9.042871	6.503418	-0.446895
121.H	7.274300	5.656308	-1.816318
122.H	8.590864	4.610143	-2.377314
123.H	7.741964	2.729705	-1.159298
124.H	5.082611	5.540506	-1.170411
125.H	2.952064	-0.556575	-1.704549
126.H	4.812036	-2.019200	-1.760461
127.H	6.424554	-1.302405	-1.655105
128.H	-5.670825	7.216949	-1.959026
129.H	-4.632770	8.558160	-2.473139
130.O	-1.221682	-10.061878	0.999887
131.H	-2.787153	7.747968	-1.176713
132.H	-5.555544	5.054724	-1.281859
133.H	0.574642	2.975244	-1.590801
134.H	2.028500	4.848503	-1.525185
135.H	1.293407	6.444547	-1.456123
136.H	-6.959128	4.271649	1.972759
137.H	-7.453764	0.421112	1.894192
138.H	4.081365	-10.052968	-0.854737
139.H	-1.388158	2.697093	1.721984
140.C	-4.502453	4.844243	-1.379796
141.N	-3.963125	3.650169	-1.526737
142.C	-2.584118	3.868106	-1.559639
143.C	-1.501569	2.951689	-1.594605

144.O	−1.554723	1.695072	−1.629210
145.N	1.182884	5.445270	−1.566097
146.N	−1.100583	5.834564	−1.423563
147.C	−2.305338	5.236614	−1.440766
148.H	−5.849892	6.215976	1.809690
149.H	−1.463931	5.057191	1.718097
150.H	10.097255	3.871749	−0.237923
151.H	−3.037946	5.835821	1.591186
152.P	−8.510676	6.377521	−0.219820
153.O	−8.908588	7.894007	0.111300
154.O	−8.798843	5.854203	−1.582415
155.O	−6.935144	6.377056	0.049233
156.C	−6.300616	7.018813	1.222130
157.N	−0.253112	3.602236	−1.556786
158.H	−8.197610	−9.887989	0.518426
159.C	−5.224649	8.009801	0.778660
160.O	−3.949475	7.351550	0.486472
161.C	−5.551361	8.815392	−0.497897
162.C	−3.339561	−7.431123	1.668034
163.N	−0.321587	−5.368647	1.567530
164.C	−1.335322	−4.421106	1.712074
165.H	−7.770790	−2.726189	−0.701547
166.C	−1.302360	−3.002308	1.720734
167.H	−1.702205	−10.728666	2.933481
168.H	−2.466543	−11.649843	1.608236
169.H	−4.096967	−10.280917	2.739404
170.H	−2.470574	−8.361201	−0.087027
171.H	−4.028651	−7.570350	−0.418668
172.H	−4.264147	−6.913440	1.930690
173.H	−0.460622	−7.510441	1.467771
174.O	−10.679792	1.454280	1.673810
175.H	−8.603877	−4.923197	2.083044
176.H	−3.027602	0.594903	−1.541297
177.H	−2.614265	−1.400184	1.835613
178.H	−4.976801	−1.458573	1.985238
179.H	−5.760720	−3.024498	1.921948
180.P	−6.556269	−8.518940	0.073134
181.O	−7.989160	−8.942230	0.651741
182.O	−6.277472	−8.756717	−1.369524
183.N	−2.424825	2.662463	1.774174
184.O	−6.507617	−6.953617	0.393668
185.C	−7.075927	−6.316646	1.600532
186.C	−7.991181	−5.159858	1.207256
187.O	−7.235576	−3.951155	0.883530
188.C	−8.879682	−5.416673	−0.019223
189.O	−10.104611	−4.665825	0.184230
190.C	−8.042509	−4.855965	−1.182829
191.O	−5.546167	−9.263690	1.081914
192.C	−10.842067	2.621450	2.515257
193.N	−5.882305	−1.061034	−1.189778
194.C	−9.722996	3.645926	2.348760
195.O	−8.451942	3.059193	2.805374
196.C	−3.462106	−8.142018	0.316641
197.C	−7.273743	−3.685644	−0.549684
198.N	−5.908986	−3.502814	−1.037087
199.C	−4.903597	−4.465644	−1.133848
200.C	−9.475774	4.113277	0.896562
201.H	−4.047750	−10.252458	−0.009963
202.O	−9.207970	5.570795	0.984738
203.C	−8.235101	3.327859	0.480703
204.C	−7.449808	3.311044	1.793972
205.N	−3.717883	−3.936843	−1.364496
206.C	−3.160537	3.837194	1.809586
207.N	−2.492476	5.004913	1.814053
208.N	−4.500593	3.849604	1.853624
209.C	−5.043453	2.621773	1.867714
210.H	−10.905705	2.329811	3.570502
211.C	−3.931478	−2.556302	−1.405558
212.C	−3.404545	−9.778221	2.056975

213.O	−3.071375	−8.469513	2.636855
214.N	−6.398879	2.318930	1.875805
215.C	−4.113451	−9.456006	0.731516
216.H	−11.788056	3.087196	2.223177
217.O	10.213346	−1.155633	1.209977
218.H	−9.952398	4.516026	2.974812
219.C	10.692601	−2.335690	1.902416
220.C	9.786354	−3.561022	1.748019
221.O	8.466598	−3.283006	2.329730
222.H	−10.335489	3.970332	0.242213
223.C	9.502783	−4.007402	0.304116
224.H	−8.539982	2.310151	0.215226
225.H	−10.662992	−4.802837	−0.602822
226.O	9.284030	−5.476370	0.372668
227.C	2.506800	−3.810542	−1.805268
228.C	1.419448	−2.900256	−1.762366
229.O	1.466051	−1.642896	−1.764860
230.N	0.178303	−3.559708	−1.682119
231.C	0.011948	−4.933160	−1.664371
232.N	−1.247746	−5.409337	−1.679277
233.N	1.042828	−5.790081	−1.655977
234.C	2.242766	−5.184010	−1.714465
235.H	5.962716	−6.250593	1.352679
236.H	7.181964	−7.559330	1.231766
237.H	5.158394	−8.700054	1.095528
238.H	6.640364	−8.874429	−1.238168
239.H	5.606166	−7.097150	−2.449647
240.H	4.562156	−8.430471	−2.971874
241.H	2.770001	−7.704723	−1.548609
242.H	5.496237	−4.979686	−1.712666
243.H	−0.653164	−2.936701	−1.657941
244.H	−2.088610	−4.817393	−1.555942
245.H	−1.348607	−6.411334	−1.586020
246.O	−5.002341	10.153377	−0.451526
247.C	−4.939183	7.951545	−1.618723
248.C	−3.736330	7.257461	−0.955233
249.C	−0.076520	4.973735	−1.507474
250.H	−7.061823	7.538186	1.807498
251.H	−5.038507	8.679008	1.624439
252.H	−4.037529	10.093834	−0.321510
253.C	−6.500683	0.928139	1.877464
254.H	8.320148	9.717184	0.520645
255.N	−3.545622	5.858702	−1.330495
256.H	−6.234695	−5.941455	2.186874
257.H	−6.624096	8.954930	−0.629005
258.H	−0.399295	−10.579844	1.047465
259.H	0.981116	9.997269	1.850304
260.H	−9.869288	8.066838	0.058529
261.N	6.437539	−2.362084	1.493278
262.C	−0.929790	−6.540676	1.561402
263.H	10.598876	−1.147083	0.316496
264.H	9.931825	−7.950792	−0.632836
265.K	−0.001137	0.000194	0.008003

GQ-**Rb**$^{+}$ (Bond Energy: -38283.5 kcal/mol)

1.C	−5.404081	−3.824443	1.337764
2.N	−4.140045	−3.449444	1.378811
3.C	−4.167209	−2.056978	1.426126
4.C	−3.116465	−1.103588	1.445226
5.O	−1.877748	−1.322352	1.433762
6.N	−3.598508	0.220290	1.462035
7.C	−4.937727	0.579310	1.475094
8.N	−5.244258	1.888949	1.518646
9.N	−5.927465	−0.325021	1.464889
10.C	−5.489634	−1.594054	1.431392
11.H	−9.552791	−5.939790	2.831679
12.H	−10.723722	−5.878723	1.492555

13.H	−10.365424	−3.652483	2.440356
14.H	−10.299257	−4.073744	−0.336874
15.H	−7.852503	−4.058534	−0.387823
16.H	−8.226586	−2.371400	−0.814659
17.H	−8.016580	−1.699123	1.570941
18.H	−5.758922	−4.843397	1.301757
19.H	−2.868777	0.958874	1.464640
20.H	−4.533019	2.633328	1.425912
21.H	−6.207496	2.129966	1.287959
22.P	−10.642197	−1.065632	−0.564485
23.O	−11.943986	−0.242375	−0.123647
24.O	−10.559940	−1.564944	−1.963912
25.O	−9.469553	−0.015215	−0.286607
26.C	−9.390267	0.833417	0.922747
27.C	1.151363	3.136990	−2.094422
28.C	−9.258496	2.306386	0.535578
29.O	−7.873029	2.680392	0.241434
30.C	−10.054345	2.734995	−0.716838
31.O	−10.546149	4.091778	−0.610887
32.C	−9.032735	2.548293	−1.856844
33.C	−7.666365	2.809948	−1.197768
34.C	4.170005	2.060980	1.421401
35.N	−6.592733	1.914401	−1.623272
36.C	3.118289	1.108480	1.441170
37.H	4.933991	1.804559	−1.943696
38.N	2.473495	2.650168	−2.035383
39.N	1.888927	5.263128	1.487144
40.H	5.610134	3.419857	−1.792818
41.C	3.602370	3.441939	−1.908075
42.H	1.511046	9.090058	−2.265891
43.O	0.191412	2.332177	−2.212792
44.H	3.216482	9.221682	−2.731961
45.C	−8.321761	−3.132704	−0.039469
46.N	−2.738567	6.295068	1.367491
47.H	−0.039544	7.533835	−1.629934
48.H	0.703963	10.278150	1.507102
49.H	2.129187	10.948058	−0.899929
50.H	8.235729	2.339992	−0.805604
51.C	−6.617491	0.521137	−1.709289
52.N	−5.421374	0.007346	−1.919089
53.O	−1.320281	1.897679	1.426955
54.C	0.578868	4.958065	1.448846
55.C	−5.600491	9.734028	1.755560
56.N	0.219638	3.619079	1.442526
57.C	−7.723447	−2.719022	1.306713
58.C	2.290241	5.261376	−1.804191
59.O	1.879743	1.327474	1.431721
60.H	7.934587	6.210293	1.236413
61.N	4.144358	3.453612	1.378612
62.N	−0.325706	5.947688	1.437840
63.C	−1.595179	5.509289	1.413626
64.N	4.801482	2.830832	−1.940393
65.O	6.245909	−8.834125	0.820794
66.C	5.598771	−9.740690	1.745604
67.C	4.077240	−9.625399	1.734801
68.O	3.685295	−8.291232	2.220826
69.C	3.423555	−9.776827	0.343435
70.O	2.187818	−10.569125	0.565269
71.C	3.110740	−8.337436	−0.057625
72.C	2.722249	−7.739655	1.296201
73.N	2.740265	−6.291955	1.367695
74.C	3.828180	−5.419366	1.338059
75.N	3.452261	−4.155564	1.379959
76.C	2.059842	−4.183464	1.418684
77.C	1.106026	−3.132957	1.433153
78.O	1.322466	−1.894222	1.424350
79.N	−0.217324	−3.615603	1.442599
80.C	−0.576808	−4.954523	1.454716
81.N	−1.886748	−5.259363	1.494997

82.N	0.327698	−5.944322	1.445199
83.C	1.597112	−5.506077	1.417479
84.H	5.963530	−9.575674	2.766432
85.H	5.873869	−10.752783	1.434147
86.H	3.665042	−10.380558	2.414020
87.H	4.045215	−10.315037	−0.371549
88.H	4.030494	−7.868479	−0.422349
89.H	2.334614	−8.240407	−0.817649
90.H	1.707331	−8.034075	1.578544
91.H	4.847593	−5.773493	1.308438
92.H	−0.954029	−2.884367	1.446037
93.H	−2.628805	−4.544445	1.407835
94.H	−2.131015	−6.220026	1.256706
95.P	1.050531	−10.672290	−0.567859
96.O	0.214968	−11.956657	−0.099239
97.O	1.552485	−10.625077	−1.967497
98.O	0.007969	−9.486463	−0.314512
99.C	−0.846100	−9.388808	0.890330
100.C	−2.317100	−9.256489	0.494694
101.O	−2.689131	−7.870373	0.201008
102.C	−2.738301	−10.049559	−0.761890
103.O	−4.096527	−10.539243	−0.666327
104.C	−2.542565	−9.025966	−1.898643
105.C	−2.809436	−7.661081	−1.238616
106.N	−1.912078	−6.585688	−1.655512
107.C	−0.518621	−6.609503	−1.737289
108.N	−0.004761	−5.411983	−1.939281
109.C	−1.097613	−4.543150	−1.977489
110.C	−1.154301	−3.130626	−2.094083
111.O	−0.194060	−2.325822	−2.213895
112.N	−2.476326	−2.644463	−2.035718
113.C	−3.605252	−3.436270	−1.909364
114.N	−4.804239	−2.825307	−1.943707
115.N	−3.546118	−4.768016	−1.774186
116.C	−2.292578	−5.255020	−1.802314
117.H	−0.521876	−8.497142	1.431469
118.H	−0.708345	−10.279816	1.505142
119.H	−2.912658	−9.555863	1.362372
120.H	−2.127158	−10.940354	−0.905024
121.H	−1.518140	−9.081144	−2.270737
122.H	−3.225438	−9.210831	−2.730630
123.H	−3.816224	−7.286298	−1.429698
124.H	0.037670	−7.526573	−1.622613
125.H	−2.579452	−1.615521	−2.118265
126.H	−4.936670	−1.798772	−1.945769
127.H	−5.613399	−3.414971	−1.801387
128.H	9.096973	−1.530374	−2.222172
129.H	9.219367	−3.239610	−2.676567
130.O	−6.244840	8.825533	0.830568
131.H	7.283403	−3.815530	−1.384278
132.H	7.535302	0.037110	−1.598539
133.H	1.623446	−2.572023	−2.121701
134.H	1.802544	−4.929227	−1.947879
135.H	3.416214	−5.609069	−1.793680
136.H	8.019076	1.701858	1.587322
137.H	5.765245	4.845892	1.305461
138.H	−9.790577	4.691768	−0.468025
139.H	2.868211	−0.953409	1.460573
140.C	6.618215	−0.518242	−1.716851
141.N	5.422757	−0.003003	−1.927391
142.C	4.552491	−1.094695	−1.967345
143.C	3.140264	−1.149109	−2.086874
144.O	2.336002	−0.188654	−2.205433
145.N	2.829158	−4.798733	−1.939942
146.N	4.772450	−3.543134	−1.758879
147.C	5.261609	−2.290399	−1.785755
148.H	8.508770	−0.515956	1.488923
149.H	4.531294	−2.630724	1.421163
150.H	−4.695784	−9.781979	−0.529972

151.H	6.205404	−2.129039	1.279690
152.P	10.656461	1.046369	−0.544288
153.O	11.948373	0.216518	−0.087613
154.O	10.590128	1.539388	−1.946806
155.O	9.475943	0.003047	−0.272280
156.C	9.390610	−0.846674	0.935871
157.N	2.651920	−2.470698	−2.033369
158.H	−0.718728	12.799370	−0.154261
159.C	9.246185	−2.317317	0.545777
160.O	7.858974	−2.677207	0.242630
161.C	10.045360	−2.751635	−0.702469
162.C	−2.721017	7.742802	1.297463
163.N	−3.450390	4.158564	1.383892
164.C	−2.057745	4.186636	1.417787
165.H	3.813545	7.294809	−1.437431
166.C	−1.103729	3.136440	1.434198
167.H	−5.963388	9.565707	2.776398
168.H	−5.880985	10.744981	1.445739
169.H	−3.669048	10.381716	2.423732
170.H	−4.036373	7.874899	−0.415816
171.H	−2.342481	8.247719	−0.817652
172.H	−1.705063	8.036728	1.576106
173.H	−4.846103	5.776065	1.316287
174.O	8.826687	6.246117	0.848608
175.H	2.907210	9.557111	1.365212
176.H	2.576120	1.621042	−2.118813
177.H	0.956393	2.887775	1.446197
178.H	2.631328	4.548434	1.402096
179.H	2.133082	6.223226	1.246636
180.P	−1.055361	10.677714	−0.562820
181.O	−0.218287	11.961723	−0.095883
182.O	−1.562607	10.633466	−1.960902
183.N	3.599146	−0.215810	1.456814
184.O	−0.012391	9.491217	−0.314667
185.C	0.842136	9.389225	0.889199
186.C	2.314018	9.258736	0.495299
187.O	2.689550	7.874162	0.198483
188.C	2.736793	10.054440	−0.758753
189.O	4.097134	10.538085	−0.662268
190.C	2.536934	9.034233	−1.898028
191.O	−2.189364	10.572144	0.573646
192.C	9.727172	5.594197	1.776132
193.N	3.543585	4.773755	−1.774041
194.C	9.611883	4.072574	1.758398
195.O	8.276979	3.677127	2.239236
196.C	−3.115150	8.342926	−0.053826
197.C	2.806761	7.667887	−1.242450
198.N	1.909798	6.592358	−1.659114
199.C	0.516480	6.616416	−1.742429
200.C	9.768166	3.424867	0.364605
201.H	−4.048864	10.322833	−0.360315
202.O	10.563594	2.190310	0.582948
203.C	8.330053	3.112501	−0.041602
204.C	7.727467	2.718453	1.308461
205.N	0.002477	5.418879	−1.944489
206.C	4.938000	−0.576310	1.468789
207.N	5.242813	−1.886163	1.511810
208.N	5.928678	0.327027	1.458082
209.C	5.492133	1.596683	1.425504
210.H	9.555742	5.954766	2.797254
211.C	1.095292	4.549755	−1.980138
212.C	−4.078238	9.626001	1.743374
213.O	−3.680078	8.292738	2.227341
214.N	6.279671	2.738429	1.374208
215.C	−3.426464	9.781436	0.351754
216.H	10.741651	5.869991	1.472730
217.O	−8.799979	−6.251250	0.895089
218.H	10.364913	3.657954	2.438279
219.C	−9.714633	−5.593139	1.804175

220.C	−9.607216	−4.071211	1.768739
221.O	−8.275997	−3.664079	2.250015
222.H	10.307086	4.050859	−0.346188
223.C	−9.760459	−3.440163	0.367257
224.H	7.861883	4.033410	−0.404378
225.H	4.690973	9.780111	−0.507027
226.O	−10.555190	−2.202583	0.570249
227.C	−4.552668	1.099993	−1.958852
228.C	−3.140992	1.155374	−2.081391
229.O	−2.337391	0.194802	−2.202386
230.N	−2.653257	2.477150	−2.029246
231.C	−3.443673	3.606499	−1.896303
232.N	−2.832192	4.805099	−1.934728
233.N	−4.774429	3.548095	−1.750781
234.C	−5.262789	2.294952	−1.777017
235.H	−8.504168	0.509673	1.473046
236.H	−10.288030	0.689682	1.526441
237.H	−9.557867	2.895704	1.407812
238.H	−10.944429	2.123396	−0.862825
239.H	−9.088344	1.526853	−2.236931
240.H	−9.219366	3.237072	−2.683441
241.H	−7.290699	3.817344	−1.383794
242.H	−7.533955	−0.034899	−1.590133
243.H	−1.624817	2.578695	−2.118394
244.H	−1.805672	4.935866	−1.947709
245.H	−3.419032	5.614055	−1.780457
246.O	10.523963	−4.113190	−0.596037
247.C	9.032156	−2.553396	−1.847985
248.C	7.660845	−2.808889	−1.197572
249.C	3.441565	−3.600665	−1.902229
250.H	10.291113	−0.712637	1.537992
251.H	9.533260	−2.910750	1.419275
252.H	9.762598	−4.706122	−0.454514
253.C	5.408995	3.827353	1.339078
254.Rb	0.000025	0.002719	−0.394763
255.H	0.721202	−12.791792	−0.136693
256.N	6.591744	−1.911464	−1.630263
257.H	0.517300	8.496092	1.427603
258.H	10.941786	−2.148122	−0.843196
259.H	−6.198650	7.934522	1.219695
260.H	6.203298	−7.943190	1.210534
261.H	12.781077	0.725640	−0.138442
262.N	−6.276184	−2.736654	1.377320
263.C	−3.826479	5.422311	1.342318
264.H	−7.912809	−6.205718	1.292836
265.H	−12.772980	−0.755313	−0.198820

GQ-**Cs**$^{+}$ (Bond Energy: -38276.8 kcal/mol)

1.C	6.461856	−1.479305	1.340828
2.N	5.343918	−0.789195	1.459755
3.C	4.327138	−1.739959	1.523977
4.C	2.921076	−1.593753	1.645625
5.O	2.260125	−0.526982	1.733362
6.N	2.254142	−2.835369	1.640878
7.C	2.876164	−4.072670	1.568513
8.N	2.104019	−5.173744	1.611279
9.N	4.207417	−4.206869	1.481357
10.C	4.861145	−3.033663	1.455566
11.H	10.865634	−3.170035	2.620335
12.H	11.548183	−4.108054	1.271034
13.H	9.666813	−5.290276	2.283820
14.H	9.841587	−4.977807	−0.507402
15.H	8.203467	−3.159261	−0.508532
16.H	7.176177	−4.563294	−0.885829
17.H	6.637071	−4.841686	1.527603
18.H	7.455528	−1.063588	1.269782
19.H	1.220058	−2.786119	1.711297

20.H	1.073402	−5.134559	1.547351
21.H	2.555146	−6.046405	1.336648
22.P	7.817071	−7.234394	−0.641847
23.O	8.086667	−8.751960	−0.204908
24.O	8.079073	−6.847060	−2.054227
25.O	6.264484	−7.060397	−0.302917
26.C	5.628067	−7.560634	0.935358
27.C	−3.129338	−1.217853	−2.211827
28.C	4.417997	−8.430853	0.599837
29.O	3.220019	−7.633654	0.323962
30.C	4.576503	−9.338184	−0.639734
31.O	3.872921	−10.593447	−0.486326
32.C	4.015903	−8.467347	−1.781937
33.C	2.945489	−7.589131	−1.108146
34.C	−4.326343	1.739862	1.524981
35.N	2.911191	−6.200492	−1.562359
36.C	−2.920448	1.593062	1.645764
37.H	−4.602291	2.514163	−1.976104
38.N	−3.627196	0.100453	−2.132265
39.N	−5.171963	−2.100762	1.565749
40.H	−6.253378	1.957639	−1.746508
41.C	−4.956817	0.432038	−1.923567
42.H	−7.850715	−4.821056	−2.232791
43.O	−1.903365	−1.416531	−2.416141
44.H	−9.075864	−3.601545	−2.625754
45.C	7.837202	−4.122627	−0.138571
46.N	−2.860633	−6.237026	1.380320
47.H	−5.632495	−5.000746	−1.599664
48.H	−8.152951	−6.347076	1.470640
49.H	−9.624944	−5.614178	−0.843835
50.H	−7.172263	4.563715	−0.885528
51.C	3.977503	−5.310222	−1.699985
52.N	3.577731	−4.082592	−1.968077
53.O	−0.526686	−2.265287	1.742456
54.C	−4.072342	−2.874710	1.546807
55.C	−3.578232	−10.682878	1.652491
56.N	−2.834140	−2.254537	1.625682
57.C	7.185358	−3.942017	1.233782
58.C	−5.457816	−1.751843	−1.778471
59.O	−2.260139	0.526082	1.733497
60.H	−9.946376	1.780411	1.079072
61.N	−5.343257	0.789181	1.462559
62.N	−4.208228	−4.206833	1.474895
63.C	−3.036395	−4.863478	1.472148
64.N	−5.284586	1.737327	−1.933860
65.O	2.444430	10.565747	0.767867
66.C	3.572766	10.679683	1.667796
67.C	4.479622	9.452797	1.655574
68.O	3.735858	8.290721	2.170442
69.C	4.998172	9.037692	0.260050
70.O	6.413644	8.637830	0.462791
71.C	4.116151	7.845471	−0.104042
72.C	3.950145	7.185126	1.266092
73.N	2.860158	6.236786	1.381911
74.C	1.484836	6.469072	1.401051
75.N	0.793448	5.350818	1.511299
76.C	1.742619	4.331015	1.547548
77.C	1.594523	2.923651	1.649829
78.O	0.527395	2.264091	1.740684
79.N	2.834893	2.253826	1.622878
80.C	4.072864	2.874665	1.545378
81.N	5.172674	2.100405	1.566876
82.N	4.208612	4.206611	1.473820
83.C	3.036570	4.863062	1.471359
84.H	3.230700	10.862105	2.693452
85.H	4.152861	11.544988	1.333168
86.H	5.333193	9.643956	2.316218
87.H	4.978432	9.847263	−0.469018
88.H	3.150399	8.221336	−0.458153

89.H	4.541750	7.186299	−0.861589
90.H	4.850993	6.630339	1.543678
91.H	1.070658	7.464810	1.352321
92.H	2.783824	1.219033	1.685415
93.H	5.133259	1.069319	1.502054
94.H	6.045199	2.552679	1.294320
95.P	7.219894	7.813348	−0.659060
96.O	8.746097	8.072555	−0.247496
97.O	6.807681	8.088431	−2.061788
98.O	7.048417	6.258144	−0.329804
99.C	7.561088	5.616548	0.900776
100.C	8.435801	4.413231	0.552604
101.O	7.642402	3.213308	0.274562
102.C	9.335960	4.583029	−0.690808
103.O	10.595019	3.884001	−0.548043
104.C	8.461840	4.024543	−1.831463
105.C	7.591968	2.946476	−1.158990
106.N	6.201181	2.910200	−1.605405
107.C	5.308282	3.975940	−1.730583
108.N	4.077967	3.575333	−1.983669
109.C	4.143707	2.181518	−2.014518
110.C	3.127667	1.213711	−2.212680
111.O	1.901930	1.412535	−2.417865
112.N	3.625733	−0.104429	−2.132458
113.C	4.955790	−0.435536	−1.925118
114.N	5.283918	−1.740962	−1.937450
115.N	5.911183	0.483619	−1.733844
116.C	5.455921	1.748432	−1.779461
117.H	6.687571	5.292626	1.471031
118.H	8.143169	6.341249	1.472905
119.H	9.036680	4.186859	1.438861
120.H	9.608307	5.625153	−0.857078
121.H	7.838698	4.820707	−2.242147
122.H	9.068297	3.606990	−2.638015
123.H	7.970237	1.935004	−1.315892
124.H	5.628664	4.997716	−1.604248
125.H	2.929458	−0.858871	−2.275334
126.H	4.601603	−2.518048	−1.976371
127.H	6.252368	−1.961486	−1.748377
128.H	−4.812543	7.846302	−2.204761
129.H	−3.590447	9.070273	−2.592695
130.O	−2.447921	−10.569273	0.754937
131.H	−1.929809	7.962160	−1.267778
132.H	−4.997597	5.628088	−1.565809
133.H	0.856297	2.929503	−2.267278
134.H	2.517026	4.598803	−1.957177
135.H	1.961646	6.245798	−1.698120
136.H	−6.635966	4.841944	1.528415
137.H	−7.455107	1.063395	1.274344
138.H	2.930507	−10.407958	−0.317044
139.H	−1.218296	2.783453	1.707879
140.C	−3.976861	5.307301	−1.698991
141.N	−3.577855	4.079392	−1.966602
142.C	−2.183632	4.143865	−1.998264
143.C	−1.215818	3.129375	−2.206805
144.O	−1.413985	1.905455	−2.424332
145.N	1.739886	5.279317	−1.895309
146.N	−0.484417	5.906464	−1.694141
147.C	−1.749241	5.452908	−1.747237
148.H	−5.305776	6.688604	1.501466
149.H	−1.070877	5.135382	1.551267
150.H	10.415031	2.938170	−0.392246
151.H	−2.553150	6.045957	1.334917
152.P	−7.811966	7.235134	−0.642754
153.O	−8.083067	8.753183	−0.208593
154.O	−8.073533	6.844772	−2.054270
155.O	−6.259179	7.062404	−0.303545
156.C	−5.621852	7.566076	0.932983
157.N	0.102561	3.625681	−2.119800

158.H	−9.020262	−9.014815	−0.331990
159.C	−4.412035	8.435184	0.593280
160.O	−3.215010	7.636605	0.317887
161.C	−4.571987	9.339108	−0.648781
162.C	−3.950991	−7.184606	1.261984
163.N	−0.793401	−5.352039	1.509190
164.C	−1.742220	−4.331972	1.548606
165.H	−7.969949	−1.934833	−1.305942
166.C	−1.593960	−2.924728	1.651581
167.H	−3.238802	−10.869025	2.678474
168.H	−4.159548	−11.545876	1.314287
169.H	−5.335688	−9.642261	2.301895
170.H	−3.153920	−8.209292	−0.469121
171.H	−4.548302	−7.174835	−0.864067
172.H	−4.851453	−6.631645	1.545027
173.H	−1.071385	−7.465417	1.344326
174.O	−10.553657	2.425743	0.676149
175.H	−9.031204	−4.184557	1.452925
176.H	−2.930782	0.854661	−2.274385
177.H	−2.782274	−1.219744	1.685997
178.H	−5.133093	−1.069497	1.504016
179.H	−6.043927	−2.553236	1.291607
180.P	−7.224923	−7.811566	−0.666933
181.O	−8.750171	−8.078486	−0.255946
182.O	−6.812180	−8.077566	−2.071173
183.N	−2.252742	2.834558	1.640517
184.O	−7.057817	−6.257451	−0.330908
185.C	−7.567384	−5.621435	0.903297
186.C	−8.436838	−4.412346	0.562403
187.O	−7.638960	−3.215760	0.282588
188.C	−9.343110	−4.574461	−0.677284
189.O	−10.595444	−3.864883	−0.528786
190.C	−8.469065	−4.021712	−1.821082
191.O	−6.415605	−8.638616	0.450590
192.C	−10.679304	3.535033	1.598107
193.N	−5.912463	−0.486990	−1.732094
194.C	−9.458955	4.450842	1.611345
195.O	−8.295708	3.709460	2.126247
196.C	−4.119759	−7.837574	−0.111308
197.C	−7.593163	−2.947209	−1.151189
198.N	−6.203572	−2.913152	−1.602013
199.C	−5.311289	−3.979448	−1.727340
200.C	−9.034449	4.993622	0.228294
201.H	−4.976780	−9.839681	−0.485688
202.O	−8.642982	6.407038	0.457854
203.C	−7.834311	4.123529	−0.138958
204.C	−7.183864	3.942209	1.234027
205.N	−4.080952	−3.579796	−1.982193
206.C	−2.874443	4.072278	1.567130
207.N	−2.102226	5.173314	1.609841
208.N	−4.205791	4.206701	1.480778
209.C	−4.860003	3.033556	1.455672
210.H	−10.864839	3.171035	2.615579
211.C	−4.145923	−2.185706	−2.014413
212.C	−4.481397	−9.453415	1.641771
213.O	−3.733795	−8.295104	2.159260
214.N	−6.231919	2.854972	1.344127
215.C	−4.999206	−9.033496	0.247212
216.H	−11.546765	4.115920	1.270714
217.O	10.551124	−2.416855	0.684540
218.H	−9.663191	5.292475	2.283280
219.C	10.679872	−3.530062	1.601543
220.C	9.461177	−4.448309	1.612567
221.O	8.296318	−3.709393	2.127409
222.H	−9.837320	4.982314	−0.508319
223.C	9.038410	−4.991115	0.228928
224.H	−8.201589	3.160608	−0.508809
225.H	−10.405927	−2.923430	−0.358098
226.O	8.649362	−6.405447	0.457351

227.C	2.183473	−4.147396	−1.996790
228.C	1.215259	−3.133304	−2.205651
229.O	1.413123	−1.909607	−2.423786
230.N	−0.103089	−3.630316	−2.119033
231.C	−0.433991	−4.957119	−1.891320
232.N	−1.739352	−5.284661	−1.892365
233.N	0.485132	−5.910294	−1.689973
234.C	1.749857	−5.456407	−1.744211
235.H	5.312550	−6.681441	1.501472
236.H	6.353387	−8.143014	1.506307
237.H	4.193535	−9.024612	1.491529
238.H	5.616385	−9.616288	−0.810844
239.H	4.812790	−7.849979	−2.199829
240.H	3.590996	−9.076124	−2.582849
241.H	1.931749	−7.964112	−1.257802
242.H	4.999032	−5.630508	−1.571186
243.H	−0.857322	−2.934694	−2.267101
244.H	−2.516195	−4.603780	−1.951067
245.H	−1.959135	−6.251708	−1.695803
246.O	−3.865740	10.593451	−0.500696
247.C	−4.014627	8.464106	−1.789455
248.C	−2.943276	7.587482	−1.114683
249.C	0.434544	4.952738	−1.894638
250.H	−6.346862	8.150151	1.502011
251.H	−4.186242	9.032152	1.482424
252.H	−2.921944	10.406880	−0.340305
253.C	−6.461332	1.479221	1.344068
254.H	9.021355	9.007607	−0.318706
255.N	−2.910052	6.197634	−1.564818
256.H	−6.692685	−5.305341	1.476053
257.H	−5.611884	9.618728	−0.818059
258.H	−1.813966	−9.954049	1.163997
259.H	1.805762	9.957191	1.179266
260.H	−9.018411	9.024803	−0.292607
261.N	6.233009	−2.854992	1.342570
262.C	−1.485263	−6.469749	1.397347
263.H	9.949800	−1.770713	1.094883
264.H	9.020183	−9.027567	−0.295745
265.Cs	−0.000086	−0.001280	−0.354385

GQ (Bond Energy: -38265.6 kcal/mol)

1.C	6.595349	−0.974072	1.209735
2.N	5.428525	−0.371002	1.348421
3.C	4.474469	−1.387262	1.318381
4.C	3.054807	−1.343508	1.421459
5.O	2.327875	−0.341903	1.597866
6.N	2.479612	−2.632076	1.314908
7.C	3.191743	−3.812881	1.199976
8.N	2.514591	−4.978368	1.186385
9.N	4.530279	−3.849279	1.133721
10.C	5.095760	−2.631932	1.180641
11.H	10.717209	−2.115619	2.636406
12.H	11.716939	−2.658969	1.269207
13.H	10.219465	−4.422031	1.992390
14.H	10.352244	−3.888147	−0.706695
15.H	8.504897	−2.255588	−0.600385
16.H	7.697763	−3.708333	−1.237479
17.H	6.922168	−4.326370	1.003973
18.H	7.566207	−0.499612	1.188427
19.H	1.438480	−2.647002	1.352836
20.H	1.482436	−5.031110	1.132371
21.H	3.048780	−5.793156	0.890275
22.P	8.532878	−6.334200	−1.113764
23.O	8.954697	−7.846980	−0.793932
24.O	8.761643	−5.813442	−2.488833
25.O	6.967266	−6.351933	−0.786397
26.C	6.380977	−6.998904	0.409661

27.C	-3.029704	-1.565762	-2.023354
28.C	5.285313	-7.989276	0.014807
29.O	3.992763	-7.336631	-0.204807
30.C	5.545993	-8.789400	-1.279748
31.O	5.007396	-10.131053	-1.205906
32.C	4.868725	-7.926947	-2.362790
33.C	3.704273	-7.232372	-1.632351
34.C	-4.495418	1.376137	1.692357
35.N	3.502559	-5.833056	-1.992484
36.C	-3.072301	1.337230	1.735652
37.H	-4.831216	2.019723	-1.721036
38.N	-3.632171	-0.296256	-1.873139
39.N	-4.913334	-2.494662	1.882854
40.H	-6.390397	1.309249	-1.330014
41.C	-4.972462	-0.087154	-1.605358
42.H	-7.446178	-5.569074	-1.819142
43.O	-1.826675	-1.653162	-2.356120
44.H	-8.733321	-4.406852	-2.191840
45.C	8.241979	-3.295537	-0.386934
46.N	-2.325152	-6.405600	1.236193
47.H	-5.175368	-5.560996	-1.339043
48.H	-7.652747	-7.172522	1.814845
49.H	-9.177241	-6.437069	-0.403015
50.H	-7.691581	3.786269	-0.702705
51.C	4.466160	-4.831861	-2.111639
52.N	3.929655	-3.636978	-2.264184
53.O	-0.272123	-2.279794	1.563965
54.C	-3.755728	-3.162692	1.682546
55.C	-2.132199	-10.617855	1.493873
56.N	-2.575990	-2.443940	1.628270
57.C	7.462849	-3.381654	0.927895
58.C	-5.274243	-2.306200	-1.449228
59.O	-2.335677	0.335459	1.864380
60.H	-10.080997	0.964730	1.653550
61.N	-5.436784	0.351119	1.739163
62.N	-3.797128	-4.497984	1.584309
63.C	-2.587063	-5.053760	1.406496
64.N	-5.427764	1.180995	-1.611124
65.O	1.541388	10.689283	0.940396
66.C	2.601808	10.873914	1.909108
67.C	3.632864	9.748478	1.900166
68.O	2.998107	8.495929	2.342723
69.C	4.249233	9.441967	0.518319
70.O	5.681413	9.146479	0.778200
71.C	3.485402	8.201500	0.061153
72.C	3.324024	7.458208	1.388689
73.N	2.305909	6.428768	1.417296
74.C	0.917534	6.560544	1.405517
75.N	0.309735	5.389771	1.451728
76.C	1.328750	4.440393	1.469679
77.C	1.277381	3.017792	1.531305
78.O	0.266298	2.289319	1.618495
79.N	2.569666	2.444764	1.500565
80.C	3.754783	3.157488	1.503924
81.N	4.915773	2.471771	1.561467
82.N	3.797420	4.498375	1.489861
83.C	2.579291	5.066690	1.457521
84.H	2.187797	10.971312	2.919731
85.H	3.105337	11.808559	1.644799
86.H	4.431022	10.003665	2.606772
87.H	4.199144	10.280604	-0.175755
88.H	2.505916	8.513838	-0.315119
89.H	3.992138	7.617615	-0.707976
90.H	4.254060	6.957481	1.671740
91.H	0.432459	7.524572	1.385160
92.H	2.593453	1.404011	1.498462
93.H	4.970071	1.446851	1.441532
94.H	5.750723	2.999697	1.308000
95.P	6.602882	8.431185	-0.329310

96.O	8.081432	8.744091	0.203035
97.O	6.270996	8.771949	-1.739374
98.O	6.493967	6.853047	-0.103484
99.C	7.012091	6.151931	1.091945
100.C	7.994734	5.052509	0.686041
101.O	7.315455	3.804542	0.335042
102.C	8.876762	5.370219	-0.541242
103.O	10.186068	4.761108	-0.439843
104.C	8.044077	4.818472	-1.716376
105.C	7.268816	3.631827	-1.114932
106.N	5.883327	3.505196	-1.555835
107.C	4.901869	4.493999	-1.649393
108.N	3.708259	3.993059	-1.904614
109.C	3.889474	2.609921	-1.961027
110.C	2.955051	1.559477	-2.185520
111.O	1.730744	1.655663	-2.425584
112.N	3.569184	0.288079	-2.125588
113.C	4.925311	0.075072	-1.957988
114.N	5.380945	-1.189645	-2.035272
115.N	5.801937	1.068536	-1.753755
116.C	5.234370	2.287894	-1.749264
117.H	6.145691	5.713202	1.591899
118.H	7.509222	6.870076	1.746251
119.H	8.610159	4.829573	1.563014
120.H	9.069564	6.438044	-0.641376
121.H	7.357583	5.587112	-2.074360
122.H	8.678492	4.503946	-2.547924
123.H	7.729221	2.668166	-1.337497
124.H	5.133631	5.536718	-1.501845
125.H	2.923777	-0.519329	-2.239431
126.H	4.776846	-2.027577	-2.118615
127.H	6.363295	-1.320905	-1.835942
128.H	-5.619615	7.258246	-2.270709
129.H	-4.544486	8.589870	-2.729544
130.O	-1.203936	-10.024040	0.552126
131.H	-2.749177	7.714154	-1.408477
132.H	-5.573991	5.079162	-1.603228
133.H	0.526389	2.915871	-2.082688
134.H	2.015757	4.780221	-1.876414
135.H	1.283552	6.357345	-1.674131
136.H	-7.030066	4.293143	1.638447
137.H	-7.572009	0.451439	1.660461
138.H	4.052401	-10.076508	-1.015046
139.H	-1.466743	2.648110	1.594411
140.C	-4.524060	4.854457	-1.699442
141.N	-4.002730	3.658463	-1.894451
142.C	-2.620849	3.850887	-1.900143
143.C	-1.557577	2.918116	-2.060716
144.O	-1.640818	1.687514	-2.267337
145.N	1.168520	5.372853	-1.875639
146.N	-1.102905	5.781234	-1.686447
147.C	-2.318264	5.204115	-1.717981
148.H	-5.897643	6.195510	1.475632
149.H	-1.522878	5.021940	1.450459
150.H	10.077679	3.797219	-0.337053
151.H	-3.087321	5.793910	1.260654
152.P	-8.508446	6.411698	-0.606630
153.O	-8.899366	7.932756	-0.285772
154.O	-8.772998	5.890326	-1.974926
155.O	-6.939095	6.399240	-0.306216
156.C	-6.327463	7.013455	0.893174
157.N	-0.293600	3.546779	-1.975890
158.H	-8.168595	-9.965851	0.115502
159.C	-5.232027	8.002101	0.494515
160.O	-3.954154	7.339183	0.226276
161.C	-5.516654	8.828913	-0.778185
162.C	-3.354161	-7.423971	1.186583
163.N	-0.328637	-5.372357	1.194866
164.C	-1.338720	-4.426119	1.363535

165.H	−7.732180	−2.703606	−0.834752
166.C	−1.284434	−3.010150	1.514038
167.H	−1.677075	−10.681782	2.490331
168.H	−2.421386	−11.628678	1.171752
169.H	−4.078520	−10.282877	2.287012
170.H	−2.483186	−8.367434	−0.561848
171.H	−4.050419	−7.598016	−0.895075
172.H	−4.279348	−6.902901	1.438883
173.H	−0.478160	−7.505387	0.974371
174.O	−10.770813	1.513555	1.240407
175.H	−8.555225	−5.009567	1.880681
176.H	−2.993086	0.514096	−2.000086
177.H	−2.600346	−1.405996	1.693710
178.H	−4.985803	−1.468742	1.784550
179.H	−5.750910	−3.032452	1.659683
180.P	−6.573164	−8.544685	−0.345922
181.O	−7.994271	−9.010974	0.229388
182.O	−6.304172	−8.730113	−1.798100
183.N	−2.507858	2.628191	1.625168
184.O	−6.554266	−6.989243	0.023324
185.C	−7.082564	−6.412492	1.277969
186.C	−7.978146	−5.214759	0.973169
187.O	−7.206555	−4.009145	0.683694
188.C	−8.912401	−5.388745	−0.233280
189.O	−10.105839	−4.610812	0.045559
190.C	−8.095246	−4.799710	−1.396673
191.O	−5.543403	−9.300181	0.632050
192.C	−10.945622	2.685831	2.072099
193.N	−5.836052	−1.085674	−1.372980
194.C	−9.812060	3.698468	1.936099
195.O	−8.561490	3.103767	2.434408
196.C	−3.474492	−8.153664	−0.154785
197.C	−7.266229	−3.685438	−0.736384
198.N	−5.912348	−3.528814	−1.257642
199.C	−4.945774	−4.514374	−1.460619
200.C	−9.515944	4.157083	0.490851
201.H	−4.035753	−10.274160	−0.458815
202.O	−9.236831	5.612575	0.583706
203.C	−8.271138	3.357438	0.115624
204.C	−7.526003	3.336884	1.451534
205.N	−3.770009	−4.007884	−1.780465
206.C	−3.229436	3.807062	1.557362
207.N	−2.551739	4.971875	1.535638
208.N	−4.570989	3.839463	1.545445
209.C	−5.130772	2.618685	1.598788
210.H	−11.044580	2.399434	3.125965
211.C	−3.948595	−2.622699	−1.768018
212.C	−3.394954	−9.770789	1.602772
213.O	−3.093455	−8.452086	2.173048
214.N	−6.490827	2.333130	1.576549
215.C	−4.108823	−9.471587	0.275360
216.H	−11.877272	3.160157	1.749360
217.O	10.249123	−1.201812	0.864410
218.H	−10.053628	4.573661	2.550381
219.C	10.700608	−2.381728	1.575362
220.C	9.782922	−3.598173	1.416682
221.O	8.457850	−3.305101	1.976165
222.H	−10.356679	4.020916	−0.188831
223.C	9.515439	−4.054022	−0.026999
224.H	−8.577699	2.342122	−0.156700
225.H	−10.686196	−4.680052	−0.734472
226.O	9.277732	−5.519568	0.056798
227.C	2.550553	−3.839505	−2.221120
228.C	1.477630	−2.907649	−2.301185
229.O	1.547372	−1.671047	−2.474465
230.N	0.222429	−3.544377	−2.168849
231.C	0.037563	−4.908857	−2.061421
232.N	−1.229530	−5.378443	−2.077799
233.N	1.051896	−5.782308	−1.985405

234.C	2.263602	−5.198268	−2.054862
235.H	5.953039	−6.199844	1.018739
236.H	7.166272	−7.519867	0.960371
237.H	5.147782	−8.663589	0.865983
238.H	6.610866	−8.922612	−1.469788
239.H	5.579121	−7.191484	−2.744077
240.H	4.515289	−8.533247	−3.199667
241.H	2.742950	−7.719012	−1.805385
242.H	5.520749	−5.049677	−2.056643
243.H	−0.605176	−2.913703	−2.197003
244.H	−2.070539	−4.787751	−1.961444
245.H	−1.330003	−6.365258	−1.877901
246.O	−4.952949	10.159666	−0.698686
247.C	−4.886160	7.973450	−1.895409
248.C	−3.714398	7.244696	−1.211864
249.C	−0.096884	4.906970	−1.832125
250.H	−7.098241	7.529156	1.468767
251.H	−5.063340	8.656578	1.355522
252.H	−3.993316	10.085242	−0.541079
253.C	−6.611945	0.944945	1.653378
254.H	10.644082	−1.210001	−0.025021
255.H	8.313585	9.693181	0.189851
256.N	−3.548455	5.846876	−1.596248
257.H	−6.224103	−6.090220	1.870832
258.H	−6.583940	8.983439	−0.934670
259.H	−0.369816	−10.521387	0.612227
260.H	0.940225	10.009156	1.291660
261.H	−9.858058	8.112909	−0.349806
262.N	6.454323	−2.359143	1.110949
263.C	−0.943025	−6.538514	1.108916
264.H	9.917832	−8.006131	−0.842585

Table S6 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of GQ_{4Na}-M^+ at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

GQ_{4Na} (Bond Energy: -38243.94 kcal/mol)			
1.C	3.249776	5.816396	1.385849
2.N	2.269350	4.941334	1.507508
3.C	2.885826	3.693400	1.536414
4.C	2.336526	2.383447	1.652210
5.O	1.137261	2.064671	1.793293
6.N	3.339917	1.386321	1.600507
7.C	4.699839	1.634841	1.539918
8.N	5.550722	0.587504	1.573985
9.N	5.209333	2.872143	1.474813
10.C	4.274698	3.835087	1.455380
11.H	6.059190	9.445595	2.853906
12.H	6.996059	9.990300	1.443229
13.H	7.816851	7.841747	2.275120
14.H	7.345877	8.251795	-0.462799
15.H	5.225092	7.097702	-0.416313
16.H	6.310147	5.781361	-0.928739
17.H	6.524663	4.995315	1.396120
18.H	3.133427	6.888316	1.325458
19.H	2.988134	0.407193	1.631729
20.H	5.237048	-0.394563	1.495190
21.H	6.511466	0.798176	1.306305
22.P	9.091789	5.651694	-0.789982
23.O	10.586702	5.584679	-0.531691
24.O	8.556857	5.934563	-2.170007
25.O	8.394837	4.241455	-0.321413
26.C	8.866908	3.515057	0.850348
27.C	0.411793	-3.314462	-1.997682
28.C	9.380764	2.122681	0.486772
29.O	8.293878	1.164943	0.252607
30.C	10.238544	2.056815	-0.791329
31.O	11.278068	1.050962	-0.697087
32.C	9.205448	1.751087	-1.890901
33.C	8.117585	0.929430	-1.174523
34.C	-2.885826	-3.693400	1.536414
35.N	6.747868	1.252583	-1.559405
36.C	-2.336526	-2.383447	1.652210
37.H	-3.583002	-3.792358	-1.807220
38.N	-0.990638	-3.455003	-1.891917
39.N	0.580733	-5.540143	1.605028
40.H	-3.457323	-5.532753	-1.604950
41.C	-1.652577	-4.660167	-1.752641
42.H	2.679794	-8.806636	-2.227408
43.O	0.920064	-2.191855	-2.209583
44.H	1.186777	-9.659126	-2.665271
45.C	6.083414	6.483085	-0.127230
46.N	5.191924	-4.486594	1.341606
47.H	3.415668	-6.746708	-1.522672
48.H	4.065668	-9.669660	1.384434
49.H	2.982298	-10.770081	-0.907698
50.H	-6.310147	-5.781361	-0.928739
51.C	6.158301	2.512832	-1.661102
52.N	4.855769	2.439129	-1.851834
53.O	2.055000	-1.122342	1.770235
54.C	1.626531	-4.687932	1.554241
55.C	9.236004	-6.243858	1.806292
56.N	1.377063	-3.327747	1.603492
57.C	5.812362	5.804169	1.214656
58.C	0.325013	-5.720351	-1.652843
59.O	-1.137261	-2.064671	1.793293
60.H	-4.364834	-8.930301	1.442891
61.N	-2.269350	-4.941334	1.507508
62.N	2.863770	-5.196822	1.484594

63.C	3.825299	−4.261323	1.448045
64.N	−2.999722	−4.647901	−1.780364
65.O	−9.404249	5.063612	0.983775
66.C	−9.236004	6.243858	1.806292
67.C	−7.855115	6.879931	1.684418
68.O	−6.842518	5.946948	2.203878
69.C	−7.407535	7.241407	0.247567
70.O	−6.733013	8.538317	0.350664
71.C	−6.476190	6.085340	−0.122924
72.C	−5.794994	5.799443	1.214485
73.N	−5.191924	4.486594	1.341606
74.C	−5.805145	3.235493	1.353179
75.N	−4.930153	2.254706	1.471331
76.C	−3.682890	2.871764	1.516035
77.C	−2.373321	2.322611	1.637623
78.O	−2.055000	1.122342	1.770235
79.N	−1.377063	3.327747	1.603492
80.C	−1.626531	4.687932	1.554241
81.N	−0.580733	5.540143	1.605028
82.N	−2.863770	5.196822	1.484594
83.C	−3.825299	4.261323	1.448045
84.H	−9.430108	6.005179	2.859052
85.H	−9.985847	6.966425	1.469521
86.H	−7.839400	7.784703	2.302743
87.H	−8.247965	7.347822	−0.441655
88.H	−7.088721	5.229193	−0.422185
89.H	−5.776124	6.323825	−0.922394
90.H	−4.986883	6.510510	1.403288
91.H	−6.876357	3.118708	1.282871
92.H	−0.397350	2.978489	1.643259
93.H	0.402626	5.230490	1.528924
94.H	−0.791678	6.502457	1.342804
95.P	−5.645375	9.100372	−0.744553
96.O	−5.579431	10.592368	−0.469984
97.O	−5.922319	8.580548	−2.131809
98.O	−4.237141	8.398344	−0.277907
99.C	−3.511602	8.861732	0.897888
100.C	−2.116777	9.371676	0.538760
101.O	−1.164320	8.282285	0.297202
102.C	−2.045768	10.238784	−0.732913
103.O	−1.033786	11.271434	−0.630309
104.C	−1.744329	9.212370	−1.839857
105.C	−0.927016	8.116663	−1.130878
106.N	−1.252867	6.750934	−1.527111
107.C	−2.513999	6.165181	−1.638793
108.N	−2.442683	4.864260	−1.841713
109.C	−1.081640	4.560141	−1.844063
110.C	−0.411793	3.314462	−1.997682
111.O	−0.920064	2.191855	−2.209583
112.N	0.990638	3.455003	−1.891917
113.C	1.652577	4.660167	−1.752641
114.N	2.999722	4.647901	−1.780364
115.N	1.014883	5.831833	−1.615701
116.C	−0.325013	5.720351	−1.652843
117.H	−3.418060	8.011581	1.579832
118.H	−4.065668	9.669660	1.384434
119.H	−1.737590	9.921942	1.406004
120.H	−2.982298	10.770081	−0.907698
121.H	−2.679794	8.806636	−2.227408
122.H	−1.186777	9.659126	−2.665271
123.H	0.147576	8.216181	−1.297564
124.H	−3.415668	6.746708	−1.522672
125.H	1.532805	2.570322	−1.970571
126.H	3.583002	3.792358	−1.807220
127.H	3.457323	5.532753	−1.604950
128.H	−8.793417	−2.685153	−2.275200
129.H	−9.648256	−1.195573	−2.719848
130.O	9.404249	−5.063612	0.983775
131.H	−8.218123	0.144816	−1.343769

132.H	−6.738798	−3.415409	−1.546793
133.H	−2.568910	1.540288	−1.977362
134.H	−3.797531	3.588868	−1.820259
135.H	−5.540315	3.459021	−1.645673
136.H	−6.524663	−4.995315	1.396120
137.H	−3.133427	−6.888316	1.325458
138.H	10.864697	0.192075	−0.489923
139.H	−2.988134	−0.407193	1.631729
140.C	−6.158301	−2.512832	−1.661102
141.N	−4.855769	−2.439129	−1.851834
142.C	−4.554642	−1.077567	−1.856462
143.C	−3.308412	−0.406122	−1.997861
144.O	−2.182785	−0.913351	−2.193062
145.N	−4.652134	3.003775	−1.810716
146.N	−5.832770	1.017033	−1.646977
147.C	−5.718153	−0.322809	−1.679011
148.H	−8.020587	−3.417091	1.536444
149.H	−5.237048	0.394563	1.495190
150.H	−0.177813	10.851227	−0.424744
151.H	−6.511466	−0.798176	1.306305
152.P	−9.091789	−5.651694	−0.789982
153.O	−10.586702	−5.584679	−0.531691
154.O	−8.556857	−5.934563	−2.170007
155.O	−8.394837	−4.241455	−0.321413
156.C	−8.866908	−3.515057	0.850348
157.N	−3.453340	0.996682	−1.900802
158.Na	12.268358	5.786405	−1.928116
159.C	−9.380764	−2.122681	0.486772
160.O	−8.293878	−1.164943	0.252607
161.C	−10.238544	−2.056815	−0.791329
162.C	5.794994	−5.799443	1.214485
163.N	4.930153	−2.254706	1.471331
164.C	3.682890	−2.871764	1.516035
165.H	−0.147576	−8.216181	−1.297564
166.C	2.373321	−2.322611	1.637623
167.H	9.430108	−6.005179	2.859052
168.H	9.985847	−6.966425	1.469521
169.H	7.839400	−7.784703	2.302743
170.H	7.088721	−5.229193	−0.422185
171.H	5.776124	−6.323825	−0.922394
172.H	4.986883	−6.510510	1.403288
173.H	6.876357	−3.118708	1.282871
174.O	−5.081552	−9.415360	0.997198
175.H	1.737590	−9.921942	1.406004
176.H	−1.532805	−2.570322	−1.970571
177.H	0.397350	−2.978489	1.643259
178.H	−0.402626	−5.230490	1.528924
179.H	0.791678	−6.502457	1.342804
180.P	5.645375	−9.100372	−0.744553
181.O	5.579431	−10.592368	−0.469984
182.O	5.922319	−8.580548	−2.131809
183.N	−3.339917	−1.386321	1.600507
184.O	4.237141	−8.398344	−0.277907
185.C	3.511602	−8.861732	0.897888
186.C	2.116777	−9.371676	0.538760
187.O	1.164320	−8.282285	0.297202
188.C	2.045768	−10.238784	−0.732913
189.O	1.033786	−11.271434	−0.630309
190.C	1.744329	−9.212370	−1.839857
191.O	6.733013	−8.538317	0.350664
192.C	−6.276618	−9.245602	1.797623
193.N	−1.014883	−5.831833	−1.615701
194.C	−6.904040	−7.861467	1.668795
195.O	−5.972921	−6.853114	2.200342
196.C	6.476190	−6.085340	−0.122924
197.C	0.927016	−8.116663	−1.130878
198.N	1.252867	−6.750934	−1.527111
199.C	2.513999	−6.165181	−1.638793
200.C	−7.246046	−7.411916	0.227886

201.H	8.247965	−7.347822	−0.441655
202.O	−8.542292	−6.734321	0.316058
203.C	−6.083414	−6.483085	−0.127230
204.C	−5.812362	−5.804169	1.214656
205.N	2.442683	−4.864260	−1.841713
206.C	−4.699839	−1.634841	1.539918
207.N	−5.550722	−0.587504	1.573985
208.N	−5.209333	−2.872143	1.474813
209.C	−4.274698	−3.835087	1.455380
210.H	−6.059190	−9.445595	2.853906
211.C	1.081640	−4.560141	−1.844063
212.C	7.855115	−6.879931	1.684418
213.O	6.842518	−5.946948	2.203878
214.N	−4.500329	−5.202298	1.357103
215.C	7.407535	−7.241407	0.247567
216.H	−6.996059	−9.990300	1.443229
217.O	5.081552	9.415360	0.997198
218.H	−7.816851	−7.841747	2.275120
219.C	6.276618	9.245602	1.797623
220.C	6.904040	7.861467	1.668795
221.O	5.972921	6.853114	2.200342
222.H	−7.345877	−8.251795	−0.462799
223.C	7.246046	7.411916	0.227886
224.H	−5.225092	−7.097702	−0.416313
225.H	0.177813	−10.851227	−0.424744
226.O	8.542292	6.734321	0.316058
227.C	4.554642	1.077567	−1.856462
228.C	3.308412	0.406122	−1.997861
229.O	2.182785	0.913351	−2.193062
230.N	3.453340	−0.996682	−1.900802
231.C	4.661071	−1.656424	−1.775558
232.N	4.652134	−3.003775	−1.810716
233.N	5.832770	−1.017033	−1.646977
234.C	5.718153	0.322809	−1.679011
235.H	8.020587	3.417091	1.536444
236.H	9.674946	4.071090	1.334255
237.H	9.938912	1.745636	1.349972
238.H	10.763104	2.996417	−0.969445
239.H	8.793417	2.685153	−2.275200
240.H	9.648256	1.195573	−2.719848
241.H	8.218123	−0.144816	−1.343769
242.H	6.738798	3.415409	−1.546793
243.H	2.568910	−1.540288	−1.977362
244.H	3.797531	−3.588868	−1.820259
245.H	5.540315	−3.459021	−1.645673
246.O	−11.278068	−1.050962	−0.697087
247.C	−9.205448	−1.751087	−1.890901
248.C	−8.117585	−0.929430	−1.174523
249.C	−4.661071	1.656424	−1.775558
250.H	−9.674946	−4.071090	1.334255
251.H	−9.938912	−1.745636	1.349972
252.H	−10.864697	−0.192075	−0.489923
253.C	−3.249776	−5.816396	1.385849
254.Na	−12.268358	−5.786405	−1.928116
255.N	−6.747868	−1.252583	−1.559405
256.H	3.418060	−8.011581	1.579832
257.H	−10.763104	−2.996417	−0.969445
258.H	8.917505	−4.339321	1.415055
259.H	−8.917505	4.339321	1.415055
260.N	4.500329	5.202298	1.357103
261.C	5.805145	−3.235493	1.353179
262.H	4.364834	8.930301	1.442891
263.Na	−5.786521	12.281845	−1.861561
264.Na	5.786521	−12.281845	−1.861561

GQ_{4Na} -**Na^+** (Bond Energy: -38261.11 kcal/mol)			
1.C	3.221010	5.716100	1.511298

2.N	2.246720	4.826766	1.526897
3.C	2.874207	3.583517	1.553601
4.C	2.348128	2.264482	1.490565
5.O	1.141350	1.919814	1.414104
6.N	3.362558	1.287767	1.498405
7.C	4.721923	1.554057	1.545813
8.N	5.578154	0.514577	1.546800
9.N	5.211836	2.798704	1.594460
10.C	4.265829	3.747456	1.576549
11.H	6.066913	9.345112	3.123202
12.H	7.014058	9.906530	1.726216
13.H	7.798912	7.723864	2.504746
14.H	7.309606	8.202813	-0.226881
15.H	5.188989	7.046317	-0.190115
16.H	6.271907	5.736730	-0.723804
17.H	6.505608	4.930700	1.597627
18.H	3.093946	6.788512	1.488653
19.H	3.016566	0.310798	1.429650
20.H	5.252907	-0.458773	1.401216
21.H	6.544595	0.738080	1.315154
22.P	9.052981	5.662931	-0.671357
23.O	10.548167	5.575076	-0.423651
24.O	8.511237	6.047399	-2.023320
25.O	8.355869	4.222620	-0.300877
26.C	8.845549	3.418924	0.813121
27.C	0.323074	-3.271073	-1.691751
28.C	9.375606	2.061287	0.349547
29.O	8.299323	1.093878	0.100944
30.C	10.185303	2.087709	-0.961417
31.O	11.249355	1.103894	-0.965576
32.C	9.116618	1.820980	-2.037059
33.C	8.079738	0.929709	-1.329967
34.C	-2.874207	-3.583517	1.553601
35.N	6.686374	1.238490	-1.641315
36.C	-2.348128	-2.264482	1.490565
37.H	-3.632351	-3.814674	-1.669161
38.N	-1.071670	-3.449419	-1.636953
39.N	0.525186	-5.577537	1.604543
40.H	-3.510501	-5.581358	-1.665584
41.C	-1.712966	-4.675444	-1.647538
42.H	2.712005	-8.716964	-2.363890
43.O	0.809498	-2.112382	-1.666192
44.H	1.244775	-9.588379	-2.847201
45.C	6.049473	6.429228	0.086549
46.N	5.117217	-4.456152	1.327902
47.H	3.394584	-6.670734	-1.582667
48.H	4.063414	-9.662204	1.257357
49.H	3.047547	-10.712897	-1.103653
50.H	-6.271907	-5.736730	-0.723804
51.C	6.067181	2.486465	-1.599058
52.N	4.754263	2.394062	-1.665406
53.O	1.898397	-1.135178	1.320852
54.C	1.557679	-4.716226	1.524877
55.C	9.191605	-6.165563	1.793019
56.N	1.281899	-3.358844	1.470720
57.C	5.785507	5.734608	1.421882
58.C	0.285600	-5.698824	-1.659734
59.O	-1.141350	-1.919814	1.414104
60.H	-4.369330	-8.878149	1.691573
61.N	-2.246720	-4.826766	1.526897
62.N	2.805640	-5.200647	1.508042
63.C	3.747224	-4.251479	1.423501
64.N	-3.055616	-4.678203	-1.681292
65.O	-9.344876	4.971547	0.987885
66.C	-9.191605	6.165563	1.793019
67.C	-7.816963	6.812683	1.661996
68.O	-6.795777	5.890980	2.186841
69.C	-7.378581	7.164609	0.219586
70.O	-6.727079	8.474263	0.301361

71.C	−6.426689	6.022420	−0.138619
72.C	−5.743395	5.759189	1.202797
73.N	−5.117217	4.456152	1.327902
74.C	−5.704024	3.196778	1.247582
75.N	−4.810662	2.228040	1.293764
76.C	−3.574077	2.860935	1.389278
77.C	−2.251116	2.340207	1.393564
78.O	−1.898397	1.135178	1.320852
79.N	−1.281899	3.358844	1.470720
80.C	−1.557679	4.716226	1.524877
81.N	−0.525186	5.577537	1.604543
82.N	−2.805640	5.200647	1.508042
83.C	−3.747224	4.251479	1.423501
84.H	−9.384950	5.940365	2.848744
85.H	−9.947659	6.875529	1.443921
86.H	−7.805784	7.723292	2.271545
87.H	−8.222772	7.245113	−0.468232
88.H	−7.023967	5.153280	−0.430692
89.H	−5.729559	6.264497	−0.939256
90.H	−4.948633	6.485283	1.391953
91.H	−6.772834	3.062444	1.170034
92.H	−0.299642	3.018673	1.458426
93.H	0.458517	5.262824	1.523530
94.H	−0.743304	6.546864	1.380978
95.P	−5.673580	9.039168	−0.825711
96.O	−5.623021	10.534864	−0.571447
97.O	−5.974116	8.495883	−2.198901
98.O	−4.245202	8.362450	−0.380852
99.C	−3.503841	8.857400	0.772540
100.C	−2.126522	9.388272	0.376891
101.O	−1.151195	8.313490	0.159007
102.C	−2.095032	10.212758	−0.924426
103.O	−1.110847	11.275037	−0.871939
104.C	−1.782086	9.156639	−2.000694
105.C	−0.930452	8.105766	−1.265492
106.N	−1.232419	6.717311	−1.605618
107.C	−2.481476	6.099749	−1.654153
108.N	−2.386398	4.788148	−1.744847
109.C	−1.019605	4.508511	−1.740934
110.C	−0.323074	3.271073	−1.691751
111.O	−0.809498	2.112382	−1.666192
112.N	1.071670	3.449419	−1.636953
113.C	1.712966	4.675444	−1.647538
114.N	3.055616	4.678203	−1.681292
115.N	1.050011	5.840990	−1.628539
116.C	−0.285600	5.698824	−1.659734
117.H	−3.381035	8.020473	1.466285
118.H	−4.063414	9.662204	1.257357
119.H	−1.748403	9.975615	1.219964
120.H	−3.047547	10.712897	−1.103653
121.H	−2.712005	8.716964	−2.363890
122.H	−1.244775	9.588379	−2.847201
123.H	0.138963	8.220999	−1.452900
124.H	−3.394584	6.670734	−1.582667
125.H	1.619119	2.565477	−1.611716
126.H	3.632351	3.814674	−1.669161
127.H	3.510501	5.581358	−1.665584
128.H	−8.667042	−2.765456	−2.346753
129.H	−9.538726	−1.328557	−2.915156
130.O	9.344876	−4.971547	0.987885
131.H	−8.200684	0.130005	−1.563863
132.H	−6.638569	−3.395142	−1.482469
133.H	−2.535969	1.616172	−1.710965
134.H	−3.788287	3.625586	−1.850156
135.H	−5.547404	3.494803	−1.919469
136.H	−6.505608	−4.930700	1.597627
137.H	−3.093946	−6.788512	1.488653
138.H	10.864485	0.223429	−0.797666
139.H	−3.016566	−0.310798	1.429650

140.C	−6.067181	−2.486465	−1.599058
141.N	−4.754263	−2.394062	−1.665406
142.C	−4.475190	−1.029750	−1.739519
143.C	−3.238744	−0.330999	−1.697411
144.O	−2.082851	−0.816942	−1.609665
145.N	−4.642903	3.041550	−1.930695
146.N	−5.808509	1.041032	−1.781907
147.C	−5.667192	−0.294044	−1.729232
148.H	−8.004938	−3.263646	1.495973
149.H	−5.252907	0.458773	1.401216
150.H	−0.241091	10.886125	−0.662604
151.H	−6.544595	−0.738080	1.315154
152.P	−9.052981	−5.662931	−0.671357
153.O	−10.548167	−5.575076	−0.423651
154.O	−8.511237	−6.047399	−2.023320
155.O	−8.355869	−4.222620	−0.300877
156.C	−8.845549	−3.418924	0.813121
157.N	−3.417567	1.064043	−1.733279
158.Na	12.253974	5.926410	−1.757277
159.C	−9.375606	−2.061287	0.349547
160.O	−8.299323	−1.093878	0.100944
161.C	−10.185303	−2.087709	−0.961417
162.C	5.743395	−5.759189	1.202797
163.N	4.810662	−2.228040	1.293764
164.C	3.574077	−2.860935	1.389278
165.H	−0.138963	−8.220999	−1.452900
166.C	2.251116	−2.340207	1.393564
167.H	9.384950	−5.940365	2.848744
168.H	9.947659	−6.875529	1.443921
169.H	7.805784	−7.723292	2.271545
170.H	7.023967	−5.153280	−0.430692
171.H	5.729559	−6.264497	−0.939256
172.H	4.948633	−6.485283	1.391953
173.H	6.772834	−3.062444	1.170034
174.O	−5.091170	−9.372817	1.265203
175.H	1.748403	−9.975615	1.219964
176.H	−1.619119	−2.565477	−1.611716
177.H	0.299642	−3.018673	1.458426
178.H	−0.458517	−5.262824	1.523530
179.H	0.743304	−6.546864	1.380978
180.P	5.673580	−9.039168	−0.825711
181.O	5.623021	−10.534864	−0.571447
182.O	5.974116	−8.495883	−2.198901
183.N	−3.362558	−1.287767	1.498405
184.O	4.245202	−8.362450	−0.380852
185.C	3.503841	−8.857400	0.772540
186.C	2.126522	−9.388272	0.376891
187.O	1.151195	−8.313490	0.159007
188.C	2.095032	−10.212758	−0.924426
189.O	1.110847	−11.275037	−0.871939
190.C	1.782086	−9.156639	−2.000694
191.O	6.727079	−8.474263	0.301361
192.C	−6.282129	−9.165943	2.062707
193.N	−1.050011	−5.840990	−1.628539
194.C	−6.885065	−7.775175	1.902000
195.O	−5.933067	−6.775166	2.414692
196.C	6.426689	−6.022420	−0.138619
197.C	0.930452	−8.105766	−1.265492
198.N	1.232419	−6.717311	−1.605618
199.C	2.481476	−6.099749	−1.654153
200.C	−7.214626	−7.350917	0.449520
201.H	8.222772	−7.245113	−0.468232
202.O	−8.506369	−6.664255	0.512177
203.C	−6.049473	−6.429228	0.086549
204.C	−5.785507	−5.734608	1.421882
205.N	2.386398	−4.788148	−1.744847
206.C	−4.721923	−1.554057	1.545813
207.N	−5.578154	−0.514577	1.546800
208.N	−5.211836	−2.798704	1.594460

209.C	−4.265829	−3.747456	1.576549
210.H	−6.066913	−9.345112	3.123202
211.C	1.019605	−4.508511	−1.740934
212.C	7.816963	−6.812683	1.661996
213.O	6.795777	−5.890980	2.186841
214.N	−4.477626	−5.118718	1.547405
215.C	7.378581	−7.164609	0.219586
216.H	−7.014058	−9.906530	1.726216
217.O	5.091170	9.372817	1.265203
218.H	−7.798912	−7.723864	2.504746
219.C	6.282129	9.165943	2.062707
220.C	6.885065	7.775175	1.902000
221.O	5.933067	6.775166	2.414692
222.H	−7.309606	−8.202813	−0.226881
223.C	7.214626	7.350917	0.449520
224.H	−5.188989	−7.046317	−0.190115
225.H	0.241091	−10.886125	−0.662604
226.O	8.506369	6.664255	0.512177
227.C	4.475190	1.029750	−1.739519
228.C	3.238744	0.330999	−1.697411
229.O	2.082851	0.816942	−1.609665
230.N	3.417567	−1.064043	−1.733279
231.C	4.641888	−1.701567	−1.810216
232.N	4.642903	−3.041550	−1.930695
233.N	5.808509	−1.041032	−1.781907
234.C	5.667192	0.294044	−1.729232
235.H	8.004938	3.263646	1.495973
236.H	9.649776	3.950229	1.329457
237.H	9.973183	1.646953	1.167980
238.H	10.682166	3.047817	−1.105017
239.H	8.667042	2.765456	−2.346753
240.H	9.538726	1.328557	−2.915156
241.H	8.200684	−0.130005	−1.563863
242.H	6.638569	3.395142	−1.482469
243.H	2.535969	−1.616172	−1.710965
244.H	3.788287	−3.625586	−1.850156
245.H	5.547404	−3.494803	−1.919469
246.O	−11.249355	−1.103894	−0.965576
247.C	−9.116618	−1.820980	−2.037059
248.C	−8.079738	−0.929709	−1.329967
249.C	−4.641888	1.701567	−1.810216
250.H	−9.649776	−3.950229	1.329457
251.H	−9.973183	−1.646953	1.167980
252.H	−10.864485	−0.223429	−0.797666
253.C	−3.221010	−5.716100	1.511298
254.Na	−12.253974	−5.926410	−1.757277
255.N	−6.686374	−1.238490	−1.641315
256.H	3.381035	−8.020473	1.466285
257.H	−10.682166	−3.047817	−1.105017
258.H	8.856296	−4.258206	1.434933
259.H	−8.856296	4.258206	1.434933
260.Na	0.000000	0.000000	0.021010
261.N	4.477626	5.118718	1.547405
262.C	5.704024	−3.196778	1.247582
263.H	4.369330	8.878149	1.691573
264.Na	−5.885327	12.243463	−1.926700
265.Na	5.885327	−12.243463	−1.926700

GQ_{4Na}-$\mathbf{K^+}$ (Bond Energy: -38264.54 kcal/mol)			
1.C	3.243675	5.764668	1.402754
2.N	2.266330	4.881516	1.474708
3.C	2.892686	3.638082	1.524551
4.C	2.358163	2.322509	1.552989
5.O	1.148358	1.984082	1.557100
6.N	3.367921	1.337638	1.555805
7.C	4.729518	1.596915	1.554918
8.N	5.581033	0.552939	1.583487

9.N	5.226409	2.840025	1.535930
10.C	4.284889	3.794064	1.503509
11.H	6.088301	9.392558	2.980014
12.H	7.022422	9.953155	1.573419
13.H	7.821899	7.777755	2.357671
14.H	7.319963	8.245111	-0.372713
15.H	5.207993	7.079581	-0.329452
16.H	6.294598	5.771902	-0.858735
17.H	6.526873	4.970721	1.463748
18.H	3.120688	6.836132	1.346245
19.H	3.024758	0.357744	1.560145
20.H	5.262782	-0.427704	1.496198
21.H	6.548140	0.765675	1.344169
22.P	9.071401	5.673922	-0.775571
23.O	10.569504	5.601742	-0.535950
24.O	8.521458	5.997797	-2.140285
25.O	8.381699	4.248754	-0.340710
26.C	8.871125	3.494633	0.807339
27.C	0.346120	-3.287255	-1.773018
28.C	9.395555	2.117229	0.402571
29.O	8.315651	1.150470	0.172886
30.C	10.225498	2.089711	-0.895313
31.O	11.281439	1.098052	-0.845013
32.C	9.172361	1.790841	-1.977789
33.C	8.116357	0.935871	-1.253934
34.C	-2.892686	-3.638082	1.524551
35.N	6.730883	1.242215	-1.599597
36.C	-2.358163	-2.322509	1.552989
37.H	-3.620852	-3.819822	-1.758257
38.N	-1.051237	-3.457830	-1.739517
39.N	0.556319	-5.584058	1.589798
40.H	-3.497937	-5.580124	-1.723081
41.C	-1.697094	-4.681430	-1.723349
42.H	2.720142	-8.740478	-2.328081
43.O	0.838444	-2.130269	-1.777432
44.H	1.250479	-9.607130	-2.814862
45.C	6.070213	6.465961	-0.050066
46.N	5.164812	-4.496604	1.398274
47.H	3.404116	-6.688803	-1.535342
48.H	4.060543	-9.679459	1.292184
49.H	3.036550	-10.735518	-1.059024
50.H	-6.294598	-5.771902	-0.858735
51.C	6.116674	2.494299	-1.628352
52.N	4.806264	2.405859	-1.737774
53.O	1.982237	-1.150183	1.554039
54.C	1.599405	-4.731507	1.553706
55.C	9.226222	-6.247522	1.842567
56.N	1.338448	-3.370291	1.555432
57.C	5.808138	5.775375	1.287766
58.C	0.298424	-5.711793	-1.679276
59.O	-1.148358	-1.984082	1.557100
60.H	-4.382181	-8.911716	1.561349
61.N	-2.266330	-4.881516	1.474708
62.N	2.843056	-5.226967	1.526459
63.C	3.795889	-4.284290	1.487542
64.N	-3.040794	-4.679358	-1.775432
65.O	-9.398006	5.055637	1.038450
66.C	-9.226222	6.247522	1.842567
67.C	-7.844917	6.879007	1.706964
68.O	-6.834091	5.950651	2.239135
69.C	-7.400853	7.216134	0.262660
70.O	-6.733626	8.518234	0.339125
71.C	-6.461236	6.060699	-0.086593
72.C	-5.781446	5.802380	1.257501
73.N	-5.164812	4.496604	1.398274
74.C	-5.763903	3.239310	1.374823
75.N	-4.879491	2.263823	1.453216
76.C	-3.637794	2.892349	1.511032
77.C	-2.321879	2.359521	1.547619

78.O	−1.982237	1.150183	1.554039
79.N	−1.338448	3.370291	1.555432
80.C	−1.599405	4.731507	1.553706
81.N	−0.556319	5.584058	1.589798
82.N	−2.843056	5.226967	1.526459
83.C	−3.795889	4.284290	1.487542
84.H	−9.417746	6.025309	2.899465
85.H	−9.975594	6.966272	1.496650
86.H	−7.824916	7.793998	2.309925
87.H	−8.242516	7.302909	−0.427706
88.H	−7.066951	5.194990	−0.371978
89.H	−5.761072	6.289505	−0.888610
90.H	−4.981643	6.524602	1.440649
91.H	−6.834643	3.113736	1.311559
92.H	−0.358347	3.027884	1.564276
93.H	0.424819	5.266514	1.507630
94.H	−0.768748	6.550911	1.348573
95.P	−5.676547	9.068233	−0.791706
96.O	−5.612791	10.565320	−0.544425
97.O	−5.984940	8.523987	−2.162553
98.O	−4.253075	8.381726	−0.347233
99.C	−3.507134	8.870915	0.806133
100.C	−2.125895	9.392143	0.410988
101.O	−1.160717	8.310256	0.184211
102.C	−2.088516	10.225205	−0.884544
103.O	−1.093952	11.277957	−0.825990
104.C	−1.786051	9.173957	−1.968027
105.C	−0.937174	8.114647	−1.241806
106.N	−1.242352	6.730570	−1.593671
107.C	−2.494111	6.116169	−1.631808
108.N	−2.404743	4.806186	−1.745147
109.C	−1.038329	4.525604	−1.768678
110.C	−0.346120	3.287255	−1.773018
111.O	−0.838444	2.130269	−1.777432
112.N	1.051237	3.457830	−1.739517
113.C	1.697094	4.681430	−1.723349
114.N	3.040794	4.679358	−1.775432
115.N	1.038584	5.847967	−1.667763
116.C	−0.298424	5.711793	−1.679276
117.H	−3.390072	8.032203	1.498579
118.H	−4.060543	9.679459	1.292184
119.H	−1.741483	9.970798	1.257124
120.H	−3.036550	10.735518	−1.059024
121.H	−2.720142	8.740478	−2.328081
122.H	−1.250479	9.607130	−2.814862
123.H	0.132846	8.229317	−1.426817
124.H	−3.404116	6.688803	−1.535342
125.H	1.603184	2.577271	−1.754192
126.H	3.620852	3.819822	−1.758257
127.H	3.497937	5.580124	−1.723081
128.H	−8.736369	−2.726033	−2.331786
129.H	−9.604176	−1.260721	−2.828763
130.O	9.398006	−5.055637	1.038450
131.H	−8.232383	0.132593	−1.446255
132.H	−6.689745	−3.403654	−1.527779
133.H	−2.576345	1.601252	−1.761505
134.H	−3.816689	3.618807	−1.779760
135.H	−5.577171	3.497781	−1.757282
136.H	−6.526873	−4.970721	1.463748
137.H	−3.120688	−6.836132	1.346245
138.H	10.886031	0.228804	−0.645980
139.H	−3.024758	−0.357744	1.560145
140.C	−6.116674	−2.494299	−1.628352
141.N	−4.806264	−2.405859	−1.737774
142.C	−4.525332	−1.039727	−1.767849
143.C	−3.286730	−0.348140	−1.770787
144.O	−2.130080	−0.841152	−1.768649
145.N	−4.676571	3.039327	−1.800764
146.N	−5.847052	1.038254	−1.683670

147.C	−5.711610	−0.298993	−1.686501
148.H	−8.031626	−3.370778	1.497688
149.H	−5.262782	0.427704	1.496198
150.H	−0.229365	10.880426	−0.611507
151.H	−6.548140	−0.765675	1.344169
152.P	−9.071401	−5.673922	−0.775571
153.O	−10.569504	−5.601742	−0.535950
154.O	−8.521458	−5.997797	−2.140285
155.O	−8.381699	−4.248754	−0.340710
156.C	−8.871125	−3.494633	0.807339
157.N	−3.456733	1.049350	−1.744518
158.Na	12.221544	5.825636	−1.966002
159.C	−9.395555	−2.117229	0.402571
160.O	−8.315651	−1.150470	0.172886
161.C	−10.225498	−2.089711	−0.895313
162.C	5.781446	−5.802380	1.257501
163.N	4.879491	−2.263823	1.453216
164.C	3.637794	−2.892349	1.511032
165.H	−0.132846	−8.229317	−1.426817
166.C	2.321879	−2.359521	1.547619
167.H	9.417746	−6.025309	2.899465
168.H	9.975594	−6.966272	1.496650
169.H	7.824916	−7.793998	2.309925
170.H	7.066951	−5.194990	−0.371978
171.H	5.761072	−6.289505	−0.888610
172.H	4.981643	−6.524602	1.440649
173.H	6.834643	−3.113736	1.311559
174.O	−5.098624	−9.409408	1.129077
175.H	1.741483	−9.970798	1.257124
176.H	−1.603184	−2.577271	−1.754192
177.H	0.358347	−3.027884	1.564276
178.H	−0.424819	−5.266514	1.507630
179.H	0.768748	−6.550911	1.348573
180.P	5.676547	−9.068233	−0.791706
181.O	5.612791	−10.565320	−0.544425
182.O	5.984940	−8.523987	−2.162553
183.N	−3.367921	−1.337638	1.555805
184.O	4.253075	−8.381726	−0.347233
185.C	3.507134	−8.870915	0.806133
186.C	2.125895	−9.392143	0.410988
187.O	1.160717	−8.310256	0.184211
188.C	2.088516	−10.225205	−0.884544
189.O	1.093952	−11.277957	−0.825990
190.C	1.786051	−9.173957	−1.968027
191.O	6.733626	−8.518234	0.339125
192.C	−6.296261	−9.210611	1.918401
193.N	−1.038584	−5.847967	−1.667763
194.C	−6.904983	−7.822036	1.758891
195.O	−5.961500	−6.818779	2.278486
196.C	6.461236	−6.060699	−0.086593
197.C	0.937174	−8.114647	−1.241806
198.N	1.242352	−6.730570	−1.593671
199.C	2.494111	−6.116169	−1.631808
200.C	−7.232234	−7.394810	0.306807
201.H	8.242516	−7.302909	−0.427706
202.O	−8.531473	−6.721207	0.368862
203.C	−6.070213	−6.465961	−0.050066
204.C	−5.808138	−5.775375	1.287766
205.N	2.404743	−4.806186	−1.745147
206.C	−4.729518	−1.596915	1.554918
207.N	−5.581033	−0.552939	1.583487
208.N	−5.226409	−2.840025	1.535930
209.C	−4.284889	−3.794064	1.503509
210.H	−6.088301	−9.392558	2.980014
211.C	1.038329	−4.525604	−1.768678
212.C	7.844917	−6.879007	1.706964
213.O	6.834091	−5.950651	2.239135
214.N	−4.499965	−5.162901	1.423285
215.C	7.400853	−7.216134	0.262660

216.H	−7.022422	−9.953155	1.573419
217.O	5.098624	9.409408	1.129077
218.H	−7.821899	−7.777755	2.357671
219.C	6.296261	9.210611	1.918401
220.C	6.904983	7.822036	1.758891
221.O	5.961500	6.818779	2.278486
222.H	−7.319963	−8.245111	−0.372713
223.C	7.232234	7.394810	0.306807
224.H	−5.207993	−7.079581	−0.329452
225.H	0.229365	−10.880426	−0.611507
226.O	8.531473	6.721207	0.368862
227.C	4.525332	1.039727	−1.767849
228.C	3.286730	0.348140	−1.770787
229.O	2.130080	0.841152	−1.768649
230.N	3.456733	−1.049350	−1.744518
231.C	4.679935	−1.696054	−1.738695
232.N	4.676571	−3.039327	−1.800764
233.N	5.847052	−1.038254	−1.683670
234.C	5.711610	0.298993	−1.686501
235.H	8.031626	3.370778	1.497688
236.H	9.677727	4.045708	1.299045
237.H	9.978029	1.729487	1.244612
238.H	10.732492	3.040280	−1.065248
239.H	8.736369	2.726033	−2.331786
240.H	9.604176	1.260721	−2.828763
241.H	8.232383	−0.132593	−1.446255
242.H	6.689745	3.403654	−1.527779
243.H	2.576345	−1.601252	−1.761505
244.H	3.816689	−3.618807	−1.779760
245.H	5.577171	−3.497781	−1.757282
246.O	−11.281439	−1.098052	−0.845013
247.C	−9.172361	−1.790841	−1.977789
248.C	−8.116357	−0.935871	−1.253934
249.C	−4.679935	1.696054	−1.738695
250.H	−9.677727	−4.045708	1.299045
251.H	−9.978029	−1.729487	1.244612
252.H	−10.886031	−0.228804	−0.645980
253.C	−3.243675	−5.764668	1.402754
254.Na	−12.221544	−5.825636	−1.966002
255.N	−6.730883	−1.242215	−1.599597
256.H	3.390072	−8.032203	1.498579
257.H	−10.732492	−3.040280	−1.065248
258.H	8.907417	−4.338083	1.476688
259.H	−8.907417	4.338083	1.476688
260.K	0.000000	0.000000	−0.090419
261.N	4.499965	5.162901	1.423285
262.C	5.763903	−3.239310	1.374823
263.H	4.382181	8.911716	1.561349
264.Na	−5.814274	12.216386	−1.981723
265.Na	5.814274	−12.216386	−1.981723

GQ_{4Na}-**Rb^+** (Bond Energy: -38259.23 kcal/mol)			
1.C	3.242115	5.790084	1.389295
2.N	2.266261	4.908297	1.493349
3.C	2.895344	3.666450	1.546700
4.C	2.361975	2.353392	1.622448
5.O	1.152039	2.017506	1.675814
6.N	3.369787	1.365642	1.612073
7.C	4.731717	1.623805	1.571295
8.N	5.582038	0.578921	1.598530
9.N	5.228080	2.866161	1.518234
10.C	4.286889	3.821391	1.492481
11.H	6.030547	9.474242	2.815859
12.H	6.978910	9.998413	1.405570
13.H	7.795347	7.862562	2.265282
14.H	7.319918	8.230447	−0.481007

15.H	5.204066	7.067060	−0.409230
16.H	6.295429	5.748625	−0.904498
17.H	6.527228	5.007861	1.437326
18.H	3.118534	6.860807	1.321863
19.H	3.031131	0.384877	1.650443
20.H	5.265086	−0.402707	1.528922
21.H	6.547401	0.788147	1.346428
22.P	9.075553	5.647066	−0.786861
23.O	10.570108	5.581708	−0.528560
24.O	8.537768	5.929329	−2.165822
25.O	8.380646	4.235044	−0.317742
26.C	8.861019	3.504994	0.848694
27.C	0.359423	−3.311810	−1.887936
28.C	9.383400	2.118203	0.476130
29.O	8.300276	1.154785	0.241904
30.C	10.236295	2.063268	−0.805830
31.O	11.284290	1.066051	−0.719705
32.C	9.201055	1.752963	−1.902332
33.C	8.125122	0.918103	−1.184048
34.C	−2.895344	−3.666450	1.546700
35.N	6.748955	1.229254	−1.562828
36.C	−2.361975	−2.353392	1.622448
37.H	−3.617624	−3.812597	−1.799957
38.N	−1.040171	−3.468116	−1.832625
39.N	0.578872	−5.580733	1.602939
40.H	−3.503796	−5.566676	−1.692688
41.C	−1.695600	−4.684861	−1.754153
42.H	2.690867	−8.778204	−2.267521
43.O	0.860135	−2.160658	−1.971005
44.H	1.213894	−9.644401	−2.732278
45.C	6.066774	6.461678	−0.113752
46.N	5.189531	−4.499676	1.396176
47.H	3.391451	−6.722071	−1.508442
48.H	4.052870	−9.670567	1.350373
49.H	3.004471	−10.754685	−0.970345
50.H	−6.295429	−5.748625	−0.904498
51.C	6.146075	2.485570	−1.632501
52.N	4.840334	2.405999	−1.793950
53.O	2.019076	−1.150936	1.671379
54.C	1.624125	−4.730778	1.574171
55.C	9.261703	−6.240185	1.757828
56.N	1.366484	−3.368637	1.611953
57.C	5.805036	5.804458	1.240652
58.C	0.292338	−5.728273	−1.674292
59.O	−1.152039	−2.017506	1.675814
60.H	−4.340834	−8.958132	1.407350
61.N	−2.266261	−4.908297	1.493349
62.N	2.866284	−5.227729	1.522220
63.C	3.821816	−4.286964	1.495736
64.N	−3.040469	−4.673119	−1.792673
65.O	−9.415515	5.059674	0.932792
66.C	−9.261703	6.240185	1.757828
67.C	−7.878830	6.876546	1.661241
68.O	−6.874906	5.949034	2.209455
69.C	−7.401940	7.226712	0.231054
70.O	−6.728285	8.523506	0.335960
71.C	−6.459875	6.070216	−0.108343
72.C	−5.805113	5.805983	1.246931
73.N	−5.189531	4.499676	1.396176
74.C	−5.791118	3.243134	1.394833
75.N	−4.909604	2.266756	1.496659
76.C	−3.667429	2.895228	1.548267
77.C	−2.354475	2.361158	1.621270
78.O	−2.019076	1.150936	1.671379
79.N	−1.366484	3.368637	1.611953
80.C	−1.624125	4.730778	1.574171
81.N	−0.578872	5.580733	1.602939
82.N	−2.866284	5.227729	1.522220
83.C	−3.821816	4.286964	1.495736

84.H	−9.476681	6.002959	2.806656
85.H	−10.003536	6.963800	1.405858
86.H	−7.877200	7.786149	2.272680
87.H	−8.227810	7.325135	−0.476511
88.H	−7.063873	5.207900	−0.407644
89.H	−5.745484	6.302048	−0.896959
90.H	−5.008928	6.528002	1.445844
91.H	−6.862127	3.120168	1.331201
92.H	−0.385888	3.030129	1.651105
93.H	0.402578	5.263517	1.530958
94.H	−0.787611	6.546095	1.350267
95.P	−5.645342	9.081951	−0.766241
96.O	−5.580590	10.575306	−0.500236
97.O	−5.926414	8.551570	−2.148433
98.O	−4.233394	8.384936	−0.300291
99.C	−3.497522	8.864055	0.863066
100.C	−2.111276	9.383960	0.484577
101.O	−1.150445	8.299524	0.246343
102.C	−2.060176	10.236910	−0.797523
103.O	−1.060395	11.282696	−0.715997
104.C	−1.756682	9.201081	−1.895331
105.C	−0.918411	8.125497	−1.180727
106.N	−1.229887	6.749384	−1.558141
107.C	−2.485979	6.145776	−1.623718
108.N	−2.405915	4.839907	−1.783941
109.C	−1.041260	4.551846	−1.811486
110.C	−0.359423	3.311810	−1.887936
111.O	−0.860135	2.160658	−1.971005
112.N	1.040171	3.468116	−1.832625
113.C	1.695600	4.684861	−1.754153
114.N	3.040469	4.673119	−1.792673
115.N	1.045984	5.852923	−1.653417
116.C	−0.292338	5.728273	−1.674292
117.H	−3.389137	8.019739	1.550069
118.H	−4.052870	9.670567	1.350373
119.H	−1.728531	9.946761	1.341996
120.H	−3.004471	10.754685	−0.970345
121.H	−2.690867	8.778204	−2.267521
122.H	−1.213894	9.644401	−2.732278
123.H	0.153436	8.236878	−1.357111
124.H	−3.391451	6.722071	−1.508442
125.H	1.590282	2.589343	−1.896957
126.H	3.617624	3.812597	−1.799957
127.H	3.503796	5.566676	−1.692688
128.H	−8.778302	−2.684881	−2.280393
129.H	−9.644842	−1.205439	−2.735962
130.O	9.415515	−5.059674	0.932792
131.H	−8.236161	0.154434	−1.356513
132.H	−6.722719	−3.391039	−1.518965
133.H	−2.587360	1.589424	−1.896979
134.H	−3.809525	3.617370	−1.792204
135.H	−5.563147	3.504002	−1.684659
136.H	−6.527228	−5.007861	1.437326
137.H	−3.118534	−6.860807	1.321863
138.H	10.879548	0.202139	−0.516379
139.H	−3.031131	−0.384877	1.650443
140.C	−6.146075	−2.485570	−1.632501
141.N	−4.840334	−2.405999	−1.793950
142.C	−4.551488	−1.041447	−1.819056
143.C	−3.310652	−0.360210	−1.890467
144.O	−2.159458	−0.861181	−1.969014
145.N	−4.670301	3.040288	−1.788610
146.N	−5.850868	1.046105	−1.651928
147.C	−5.727216	−0.292292	−1.677485
148.H	−8.016991	−3.398046	1.536259
149.H	−5.265086	0.402707	1.528922
150.H	−0.196323	10.876087	−0.517149
151.H	−6.547401	−0.788147	1.346428
152.P	−9.075553	−5.647066	−0.786861

153.O	−10.570108	−5.581708	−0.528560
154.O	−8.537768	−5.929329	−2.165822
155.O	−8.380646	−4.235044	−0.317742
156.C	−8.861019	−3.504994	0.848694
157.N	−3.466407	1.039485	−1.833743
158.Na	12.268802	5.828563	−1.899615
159.C	−9.383400	−2.118203	0.476130
160.O	−8.300276	−1.154785	0.241904
161.C	−10.236295	−2.063268	−0.805830
162.C	5.805113	−5.805983	1.246931
163.N	4.909604	−2.266756	1.496659
164.C	3.667429	−2.895228	1.548267
165.H	−0.153436	−8.236878	−1.357111
166.C	2.354475	−2.361158	1.621270
167.H	9.476681	−6.002959	2.806656
168.H	10.003536	−6.963800	1.405858
169.H	7.877200	−7.786149	2.272680
170.H	7.063873	−5.207900	−0.407644
171.H	5.745484	−6.302048	−0.896959
172.H	5.008928	−6.528002	1.445844
173.H	6.862127	−3.120168	1.331201
174.O	−5.066943	−9.419783	0.952287
175.H	1.728531	−9.946761	1.341996
176.H	−1.590282	−2.589343	−1.896957
177.H	0.385888	−3.030129	1.651105
178.H	−0.402578	−5.263517	1.530958
179.H	0.787611	−6.546095	1.350267
180.P	5.645342	−9.081951	−0.766241
181.O	5.580590	−10.575306	−0.500236
182.O	5.926414	−8.551570	−2.148433
183.N	−3.369787	−1.365642	1.612073
184.O	4.233394	−8.384936	−0.300291
185.C	3.497522	−8.864055	0.863066
186.C	2.111276	−9.383960	0.484577
187.O	1.150445	−8.299524	0.246343
188.C	2.060176	−10.236910	−0.797523
189.O	1.060395	−11.282696	−0.715997
190.C	1.756682	−9.201081	−1.895331
191.O	6.728285	−8.523506	0.335960
192.C	−6.255510	−9.259493	1.764247
193.N	−1.045984	−5.852923	−1.653417
194.C	−6.882970	−7.873414	1.658099
195.O	−5.950848	−6.872943	2.204747
196.C	6.459875	−6.070216	−0.108343
197.C	0.918411	−8.125497	−1.180727
198.N	1.229887	−6.749384	−1.558141
199.C	2.485979	−6.145776	−1.623718
200.C	−7.225392	−7.401791	0.223922
201.H	8.227810	−7.325135	−0.476511
202.O	−8.523146	−6.728896	0.319716
203.C	−6.066774	−6.461678	−0.113752
204.C	−5.805036	−5.804458	1.240652
205.N	2.405915	−4.839907	−1.783941
206.C	−4.731717	−1.623805	1.571295
207.N	−5.582038	−0.578921	1.598530
208.N	−5.228080	−2.866161	1.518234
209.C	−4.286889	−3.821391	1.492481
210.H	−6.030547	−9.474242	2.815859
211.C	1.041260	−4.551846	−1.811486
212.C	7.878830	−6.876546	1.661241
213.O	6.874906	−5.949034	2.209455
214.N	−4.499038	−5.189044	1.391447
215.C	7.401940	−7.226712	0.231054
216.H	−6.978910	−9.998413	1.405570
217.O	5.066943	9.419783	0.952287
218.H	−7.795347	−7.862562	2.265282
219.C	6.255510	9.259493	1.764247
220.C	6.882970	7.873414	1.658099
221.O	5.950848	6.872943	2.204747

222.H	−7.319918	−8.230447	−0.481007
223.C	7.225392	7.401791	0.223922
224.H	−5.204066	−7.067060	−0.409230
225.H	0.196323	−10.876087	−0.517149
226.O	8.523146	6.728896	0.319716
227.C	4.551488	1.041447	−1.819056
228.C	3.310652	0.360210	−1.890467
229.O	2.159458	0.861181	−1.969014
230.N	3.466407	−1.039485	−1.833743
231.C	4.682613	−1.695448	−1.752686
232.N	4.670301	−3.040288	−1.788610
233.N	5.850868	−1.046105	−1.651928
234.C	5.727216	0.292292	−1.677485
235.H	8.016991	3.398046	1.536259
236.H	9.666582	4.063835	1.333337
237.H	9.946963	1.739941	1.335152
238.H	10.752161	3.007792	−0.983046
239.H	8.778302	2.684881	−2.280393
240.H	9.644842	1.205439	−2.735962
241.H	8.236161	−0.154434	−1.356513
242.H	6.722719	3.391039	−1.518965
243.H	2.587360	−1.589424	−1.896979
244.H	3.809525	−3.617370	−1.792204
245.H	5.563147	−3.504002	−1.684659
246.O	−11.284290	−1.066051	−0.719705
247.C	−9.201055	−1.752963	−1.902332
248.C	−8.125122	−0.918103	−1.184048
249.C	−4.682613	1.695448	−1.752686
250.H	−9.666582	−4.063835	1.333337
251.H	−9.946963	−1.739941	1.335152
252.H	−10.879548	−0.202139	−0.516379
253.C	−3.242115	−5.790084	1.389295
254.Na	−12.268802	−5.828563	−1.899615
255.N	−6.748955	−1.229254	−1.562828
256.H	3.389137	−8.019739	1.550069
257.H	−10.752161	−3.007792	−0.983046
258.H	8.963684	−4.326753	1.386596
259.H	−8.963684	4.326753	1.386596
260.Rb	0.000000	0.000000	−0.126535
261.N	4.499038	5.189044	1.391447
262.C	5.791118	−3.243134	1.394833
263.H	4.340834	8.958132	1.407350
264.Na	−5.802864	12.290706	−1.854601
265.Na	5.802864	−12.290706	−1.854601

Table S7. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of guanine, Guanosine dimer (Guanosine Monophosphate + Guanosine) and $(H_2CO)_8$ at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

Guanine in C1 (Bond Energy -2485.4 kcal/mol)			
1.N	−3.070455	2.089073	0.003575
2.N	0.473082	3.876531	−0.026013
3.C	0.469689	2.497443	−0.030280
4.N	−0.648496	1.777774	−0.016228
5.C	−1.770827	2.538345	−0.008431
6.C	−1.870419	3.939136	−0.006587
7.C	−0.671636	4.714225	−0.016552
8.C	−3.892267	3.201024	0.010659
9.N	−3.209412	4.334601	0.004709
10.O	−0.534967	5.954516	−0.017769
11.N	1.679385	1.875977	−0.097841
12.H	−4.968233	3.109411	0.020107
13.H	1.683894	0.884378	0.111746
14.H	2.510042	2.388219	0.173912
15.H	1.366767	4.362216	−0.046268
16.H	−3.368988	1.120132	0.003716

Guanosine dimer (Guanosine Monophosphate + Guanosine) (Bond Energy: -9550.84 kcal/mol)			
1.C	−9.039561	−5.059282	0.189235
2.O	−3.037938	−7.813481	2.664080
3.O	−10.104804	−4.122796	0.496910
4.C	−8.194572	−4.603585	−1.013290
5.O	−5.489670	−8.965568	1.278198
6.H	−6.497912	−6.146132	2.339812
7.N	−5.075623	−1.476502	−0.712355
8.C	−4.050829	−9.078673	0.913890
9.H	−6.043629	−2.714978	2.234892
10.C	−3.509266	−7.777830	0.333896
11.H	−0.278316	−9.946231	1.253333
12.C	−7.141489	−3.661990	−0.401521
13.N	−5.802002	−3.796413	−0.977666
14.C	−5.149780	−4.946516	−1.425834
15.C	−1.087241	−5.841070	1.151768
16.O	−1.132177	−9.487469	1.166958
17.H	−3.934559	−9.946335	0.264300
18.C	−3.701596	−3.357597	−1.559601
19.H	−7.946273	−10.100787	0.837499
20.O	−6.852532	−6.927031	0.431955
21.C	−7.350892	−6.324100	1.680504
22.N	−3.901808	−4.719943	−1.788428
23.C	−3.395022	−6.907761	1.587119
24.N	−0.549886	−4.632962	1.144551
25.C	−1.591812	−3.768926	1.498536
26.H	−7.403089	−2.608598	−0.512996
27.C	−2.549246	−2.540711	−1.765923
28.C	−1.638112	−2.347808	1.631773
29.H	−1.522789	−9.934086	3.183145
30.H	−2.264339	−11.054314	2.006363
31.H	−3.948533	−9.656996	3.002593
32.H	−2.520656	−7.974055	−0.087417
33.H	−4.136928	−7.332765	−0.436072
34.P	−6.604009	−8.489626	0.221911
35.H	−4.345416	−6.424034	1.824765
36.C	−8.050237	−5.007990	1.363496
37.H	−3.218878	1.173784	−0.543909
38.N	−2.805640	−1.198960	−1.372630
39.N	−5.240413	−2.142737	2.507674

40.H	−4.881105	0.953701	−0.109356
41.C	−3.999756	−0.712391	−0.882955
42.H	−7.726626	−5.471334	−1.479557
43.O	−1.430497	−2.848496	−2.220496
44.H	−8.797567	−4.091306	−1.766568
45.H	−0.575399	−6.769210	0.937934
46.N	−2.436818	−5.821549	1.502130
47.H	−5.648665	−5.901237	−1.461434
48.H	−8.057104	−7.009661	2.155336
49.H	−9.451453	−6.063153	0.041244
50.C	−3.300308	−9.197152	2.249791
51.O	−7.107183	−3.950234	1.023015
52.H	−8.562828	−4.695401	2.279246
53.O	−0.730826	−1.506286	1.477926
54.C	−4.051009	−2.724518	2.173374
55.C	−2.007628	−10.002799	2.200914
56.N	−2.950744	−1.913593	1.978139
57.H	−2.021967	−0.560222	−1.484789
58.C	−4.871547	−2.770018	−1.055198
59.H	−10.717199	−4.121534	−0.261345
60.O	−7.948616	−9.123342	0.823463
61.O	−6.276870	−8.765269	−1.204336
62.N	−3.986792	−4.045666	2.073639
63.C	−2.766083	−4.497570	1.728652
64.N	−4.056853	0.609425	−0.584309
65.H	−3.054998	−0.907134	2.084067
66.H	−5.348336	−1.156899	2.295947

Formaldehyde octamer (Bond Energy: -3945.2 kcal/mol)			
1.O	−0.165011	−2.345307	1.843325
2.H	−2.165411	−2.746303	1.645960
3.H	2.157197	2.752653	1.620574
4.O	−2.055226	−1.163620	−1.991441
5.H	−3.477573	0.293495	−1.752438
6.H	−0.979831	−4.231589	1.657808
7.C	−1.129117	−3.131560	1.720497
8.H	4.067496	1.504011	−1.657211
9.H	1.510569	−4.062716	−1.655022
10.C	0.785429	−3.235219	−1.813852
11.H	−4.061604	−1.512125	−1.656680
12.C	−3.233116	−0.786319	−1.806803
13.H	3.485864	−0.301748	−1.763353
14.C	3.128228	−1.121462	1.706740
15.H	4.228993	−0.973353	1.654726
16.C	3.239784	0.778045	−1.810934
17.O	−2.348588	0.162651	1.815125
18.H	−2.751227	2.164448	1.640369
19.O	2.341519	−0.156160	1.812102
20.O	1.163437	−2.057674	−1.998144
21.H	−0.294630	−3.480700	−1.769504
22.H	−4.237154	0.979755	1.670046
23.C	−3.135981	1.127779	1.712116
24.H	2.743473	−2.158669	1.643101
25.O	−1.153862	2.050204	−1.966304
26.H	0.303853	3.476548	−1.759094
27.O	0.154338	2.348862	1.776631
28.H	0.971868	4.238022	1.646552
29.C	1.119658	3.136606	1.684021
30.H	−1.501355	4.058777	−1.645832
31.C	−0.776185	3.229707	−1.795760
32.O	2.061399	1.154925	−1.992586