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Supporting Information

RNA versus DNA G-Quadruplex: The Origin of Increased Stability

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Supporting Information for

RNA vs DNA G-Quadruplex: the origin of increased stability

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Table S1 Partitioning of the bond energy energy (kcal/mol) of the final complex from the empty scaffold + cation with 4 Na^+ as counterions

Figure S1. Energy plot of the conformational search over 600 possible conformers of RNA dimer (a) and DNA dimer (b). (Energy expressed in Hartrees)

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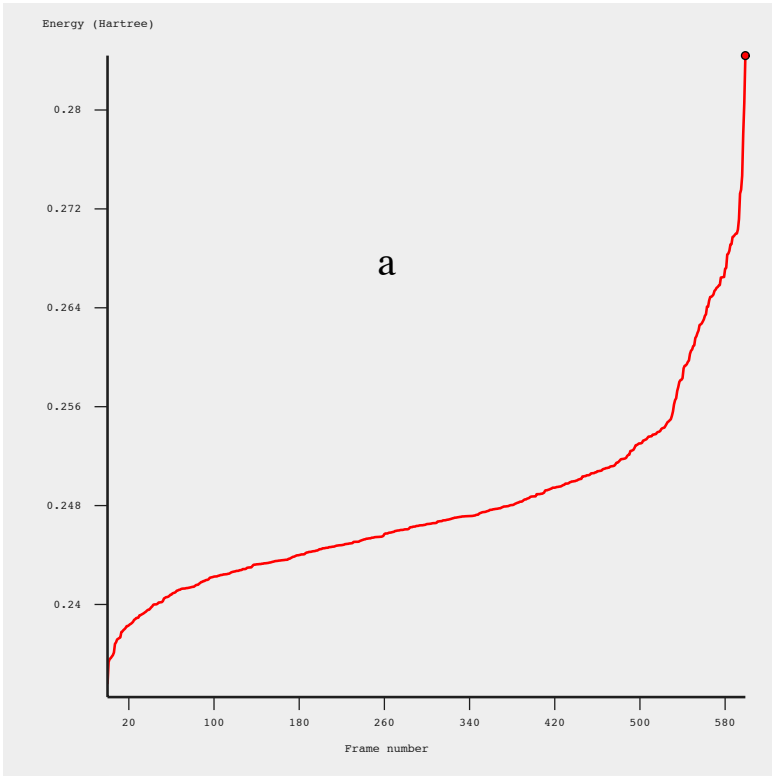
Table S6 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of guanosine dimer (guanosine monophosphate + guanosine), guanosine dimer counterion (Na^+) and $(H_2CO)_8$ at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

Table S1. Partitioning of the formation energy (kcal/mol) of the final complex from 4 Guanosine dimers with 4 Na^+ as counterions

System	M^+	ΔE_{Bond}	ΔE_{desolv}	ΔE_{prep}	ΔE_{int}	ΔE_{solv}	ΔE_{desolv} $+\Delta E_{solv}$
$_{RNA}$GQ-M^+	Na^+	-125.8	314.3	9.4	-171.1	-208.0	106.3
	K^+	-126.7	296.6	4.6	-149.0	-208.5	88.2

Figure S1. Energy plots of the conformational search over 600 possible conformers of RNA dimer (a) and DNA dimer (b). (UFF energy expressed in Hartree). ADF "conformers" module generates 600 random conformations and filters them with an RMS (0.2 Å) filter to avoid duplicate structures. Next it optimizes with RDKit-UFF so each conformation runs into some local minimum (conformer), and again filters with an RMS filter (0.1 Å) to avoid duplicate structures. The two geometries of minimum energy have been furtherly optimized at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory. The conformation for G-DNA optimized through this procedure confirmed our previous obtained geometry for G-DNA published in PCCP (F. Zaccaria, G. Paragi, C. Fonseca Guerra, *Phys. Chem. Chem. Phys.* **2016**, *18*, 20895–20904.)



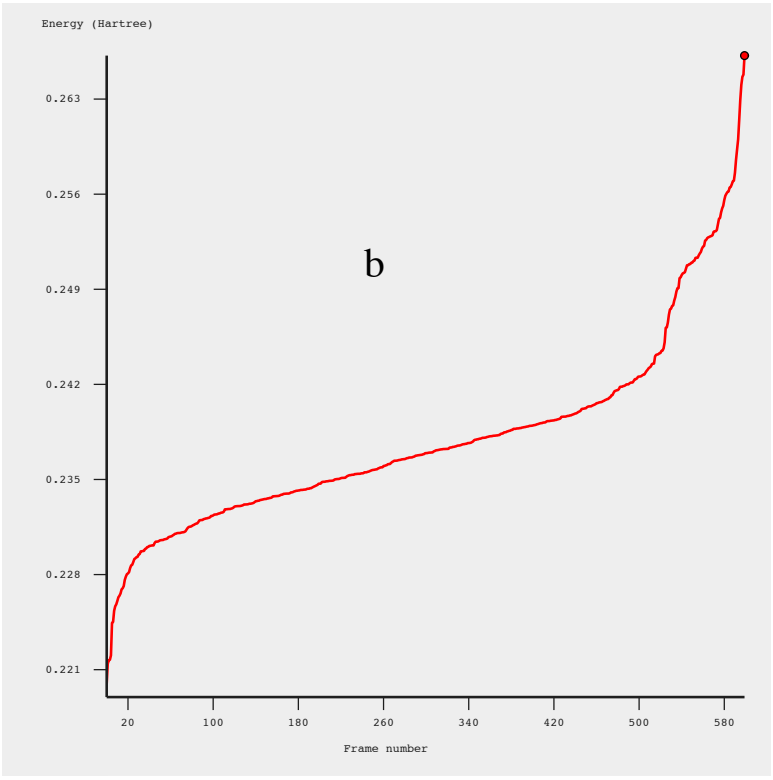


Table S2. Partitioning of the bonding energy upon formation of the final GQ-M^+complex from the empty scaffold (kcal/mol) [a]

	M^+	ΔE_{Bond}	ΔE_{Dehyd}	ΔE_{prep}	ΔE_{int}	ΔE_{Hyd}	$\Delta E_{Dehyd+Hyd}$
$_{RNA}$-GQ[ ]	Li^+	-37.1	272.7	9.8	-173.4	-146.2	126.5
	Na^+	-51.3	246.7	9.6	-161.8	-145.8	100.9
	K^+	-51.7	229.0	5.8	-139.0	-147.5	81.5
	Rb^+	-46.3	224.9	4.6	-126.9	-149.0	75.9
	Cs^+	-38.6	218.9	5.5	-112.4	-150.7	68.3
$_{DNA}$-GQ[ ]	Li^+	-37.9	251.8	11.3	-165.7	-135.2	116.5
	Na^+	-52.2	225.8	10.4	-156.6	-131.8	94.0
	K^+	-53.2	208.1	5.7	-134.7	-132.2	75.9
	Rb^+	-48.8	204.0	0.9	-119.1	-134.6	69.4
	Cs^+	-40.9	198.1	1.8	-104.4	-136.3	61.7

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

Table S3. Energy Decomposition Analysis of the interaction energy (kcal/mol) between the alkali-metal cations and the empty scaffold. [a]

	M^+	ΔE^2_{int}	ΔE^2_{Pauli}	ΔV^2_{elstat}	ΔE^2_{oi}	ΔE^2_{disp}
$_{RNA}$-GQ[ ]	Li^+	-173.4	12.5	-120.3	-57.9	-7.8
	Na^+	-161.8	11.2	-114.7	-45.3	-13.1
	K^+	-138.9	28.9	-109.6	-43.0	-15.2
	Rb^+	-126.5	36.5	-103.8	-40.7	-16.4
	Cs^+	-112.1	39.4	-95.8	-39.6	-16.1
$_{DNA}$-GQ[ ]	Li^+	-165.7	13.2	-112.8	-58.3	-7.7
	Na^+	-156.6	11.1	-109.3	-45.2	-13.1
	K^+	-134.7	29.9	-106.2	-43.2	-15.2
	Rb^+	-119.1	35.2	-97.1	-40.9	-16.5
	Cs^+	-104.4	39.1	-88.0	-39.4	-16.1

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

Table S4. Energy decomposition analysis of ΔE_{int} of 8 H_2O or 8 H_2 molecules interacting with K^+. –OH moieties are frozen in the same geometry they assume in Ribosidic 2'-OH RNA-GQ-K^+ complex (Figure 9a), while the second H is fully relaxed. In the H_2 case, the oxygens of the ribosidic 2'-OH in RNA-GQ-K^+ complex are replaced at exactly the same position in space by hydrogens (Figure 9b), and the position of the second hydrogen atom is optimized.

System	M^+	ΔE_{int}	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}	ΔE_{disp}
H_2O	K^+	-11.3	0.0	-11.0	-0.3	-0.1
H_2	K^+	-0.4	0.0	-0.2	-0.1	-0.1

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

Table S5. Relationship between the term $\Delta E_{desolv} + \Delta E_{solv}$ and ΔG_{hyd} of involved cations

System	M^+	$\Delta E_{desolv} + \Delta E_{solv}$	System	M^+	$\Delta E_{desolv} + \Delta E_{solv}$	Experimental[a] ΔG_{hyd}
$_{RNA}$GQ-M^+	Li^+	126.5	$_{DNA}$GQ-M^+	Li^+	116.5	-113.4
	Na^+	100.9		Na^+	94.0	-87.2
	K^+	81.5		K^+	75.9	-70.5
	Rb^+	75.9		Rb^+	69.4	-65.7
	Cs^+	68.3		Cs^+	61.7	-59.7

[a] Marcus, Y. (1991). Thermodynamics of Solvation of Ions, 87(18), 2995–2999

As it becomes apparent in Table S5, the difference between desolvation of the empty scaffold individually optimized plus the ion and rehydration of the fully optimized GQ-M^+ complex follows the ΔG_{Hyd} of concerned cations, so both the DNA and RNA complexes are affected by the screening effect generated by the COSMO solvation to the same extent. For this reason, although the gasphase picture overestimates the electrostatic attraction exerted by 2'-OHs over the involved cations, we can assume that the same effect concerns both models b and c in Fig. 8 (simplified models of $_{RNA}$GQ-K^+ complex where 2-OHs are substituted by H_2O or H_2) in such a way that their comparison offers a valid prediction of the differences in terms of ΔV_{elstat}.

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

$_{RNA}$GQ (Bond Energy: -39418.23) (symmetry C2)

1.C	−4.841032	−4.585151	1.427223
2.N	−3.639077	−4.046266	1.500392
3.C	−3.846593	−2.669167	1.548203
4.C	−2.923026	−1.584300	1.612431
5.O	−1.677766	−1.639309	1.683388
6.N	−3.581671	−0.331710	1.596406
7.C	−4.952986	−0.159647	1.616025
8.N	−5.447017	1.095056	1.688094
9.N	−5.815225	−1.185205	1.591219
10.C	−5.214559	−2.383083	1.532440
11.H	−8.893540	−6.943211	3.163517
12.H	−10.026786	−7.132350	1.804308
13.H	−9.864029	−4.794085	2.481003
14.H	−9.679473	−5.509898	−0.226283
15.H	−7.246470	−5.376073	−0.124629
16.O	−7.553471	−3.547213	−1.078758
17.H	−7.696016	−2.769975	1.431431
18.H	−5.060066	−5.641959	1.370803
19.H	−2.952149	0.498729	1.601626
20.H	−4.870248	1.945884	1.575205
21.H	−6.446849	1.173257	1.522799
22.P	−10.559134	−2.759648	−0.830675
23.O	−12.125375	−2.541482	−0.596423
24.O	−10.132207	−3.333057	−2.140993
25.O	−10.005035	−1.265207	−0.656224
26.C	−10.255728	−0.472307	0.572374
27.C	0.690750	3.243043	−2.044596
28.C	−9.820281	0.967439	0.356414
29.O	−8.364963	1.055568	0.304493
30.C	−10.344683	1.657922	−0.928026
31.O	−10.764007	3.015975	−0.683426
32.C	−9.149188	1.580277	−1.914940
33.C	−7.928698	1.638455	−0.950039

34.C	3.846593	2.669167	1.548203
35.N	−6.739992	0.935738	−1.377554
36.C	2.923026	1.584300	1.612431
37.H	4.615479	2.449372	−1.797435
38.N	2.070049	2.944383	−1.955411
39.N	1.094568	5.449651	1.696418
40.H	5.068309	4.118920	−1.568756
41.C	3.071751	3.882612	−1.773092
42.O	0.418512	9.181040	−2.742467
43.O	−0.140701	2.345611	−2.301209
44.H	2.442669	9.138009	−2.575826
45.C	−7.765842	−4.418329	0.022882
46.N	−3.618596	5.854340	1.446968
47.H	−1.149387	7.359226	−1.260132
48.H	−0.498684	11.327912	0.804945
49.H	1.154229	11.215791	−1.337847
50.O	7.553471	3.547213	−1.078758
51.C	−6.568221	−0.446401	−1.468965
52.N	−5.321596	−0.769119	−1.748809
53.O	−1.641432	1.682350	1.688147
54.C	−0.160333	4.956851	1.620560
55.C	−6.737304	9.048595	2.099654
56.N	−0.333205	3.585791	1.597665
57.C	−7.275267	−3.777803	1.330643
58.C	1.511870	5.488253	−1.591163
59.O	1.677766	1.639309	1.683388
60.H	7.193636	7.271831	1.703231
61.N	3.639077	4.046266	1.500392
62.N	−1.185543	5.819447	1.595493
63.C	−2.383677	5.219608	1.531882
64.N	4.348608	3.452557	−1.820617
65.O	7.426319	−8.060164	1.299836
66.C	6.737304	−9.048595	2.099654
67.C	5.227251	−9.058624	1.884899
68.O	4.660281	−7.779807	2.354313
69.C	4.768447	−9.216041	0.419429
70.O	3.568123	−10.080124	0.466784
71.C	4.419550	−7.773368	0.022603
72.C	3.776573	−7.281520	1.328874
73.N	3.618596	−5.854340	1.446968
74.C	4.585574	−4.847119	1.422705
75.N	4.047454	−3.644893	1.496112
76.C	2.670412	−3.851733	1.546563
77.C	1.586184	−2.927653	1.614022
78.O	1.641432	−1.682350	1.688147
79.N	0.333205	−3.585791	1.597665
80.C	0.160333	−4.956851	1.620560
81.N	−1.094568	−5.449651	1.696418
82.N	1.185543	−5.819447	1.595493
83.C	2.383677	−5.219608	1.531882
84.H	6.941924	−8.892831	3.165799
85.H	7.136944	−10.023867	1.805713
86.H	4.798275	−9.871257	2.482082
87.H	5.510601	−9.688451	−0.223519
88.H	5.378080	−7.255053	−0.123027
89.O	3.552104	−7.558916	−1.081745
90.H	2.768020	−7.700950	1.427141
91.H	5.642214	−5.066161	1.362945
92.H	−0.496793	−2.956101	1.601080
93.H	−1.944639	−4.872077	1.581057
94.H	−1.174051	−6.449618	1.533674
95.P	2.754024	−10.562642	−0.825038
96.O	2.531443	−12.128905	−0.598326
97.O	3.323825	−10.130785	−2.135621
98.O	1.262127	−10.004888	−0.643710
99.C	0.467459	−10.258932	0.582930
100.C	−0.970289	−9.818079	0.364332
101.O	−1.051873	−8.362637	0.310344
102.C	−1.659416	−10.342134	−0.921501
103.O	−3.017282	−10.762662	−0.679163
104.C	−1.579925	−9.146173	−1.907883
105.C	−1.637654	−7.926115	−0.942769
106.N	−0.935523	−6.737334	−1.370421
107.C	0.446592	−6.565269	−1.460135
108.N	0.769415	−5.318247	−1.737816
109.C	−0.436122	−4.624175	−1.816075
110.C	−0.690750	−3.243043	−2.044596
111.O	0.140701	−2.345611	−2.301209
112.N	−2.070049	−2.944383	−1.955411
113.C	−3.071751	−3.882612	−1.773092
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115.N	−2.823220	−5.188598	−1.586003
116.C	−1.511870	−5.488253	−1.591163
117.H	0.920704	−9.688747	1.396859
118.H	0.498684	−11.327912	0.804945
119.H	−1.529540	−10.160935	1.243051
120.H	−1.154229	−11.215791	−1.337847
121.O	−0.418512	−9.181040	−2.742467
122.H	−2.442669	−9.138009	−2.575826
123.H	−2.680438	−7.626529	−0.784898
124.H	1.149387	−7.359226	−1.260132
125.H	−2.309535	−1.938157	−2.067453
126.H	−4.615479	−2.449372	−1.797435
127.H	−5.068309	−4.118920	−1.568756
128.O	9.183652	−0.419926	−2.751059
129.H	9.142359	−2.443820	−2.581786
130.O	−7.426319	8.060164	1.299836
131.H	7.628622	−2.681290	−0.794073
132.H	7.361729	1.149448	−1.267998
133.H	1.940126	−2.308896	−2.071777
134.H	2.450966	−4.614050	−1.793023
135.H	4.120733	−5.066385	−1.565172
136.H	7.696016	2.769975	1.431431
137.H	5.060066	5.641959	1.370803
138.H	−10.060809	3.491071	−0.202415
139.H	2.952149	−0.498729	1.601626
140.C	6.568221	0.446401	−1.468965
141.N	5.321596	0.769119	−1.748809
142.C	4.627363	−0.436376	−1.826560
143.C	3.247179	−0.691344	−2.060590
144.O	2.351634	0.139469	−2.327449
145.N	3.454291	−4.348542	−1.822102
146.N	5.190795	−2.823206	−1.591767
147.C	5.490860	−1.512018	−1.598334
148.H	9.680618	0.924767	1.383272
149.H	4.870248	−1.945884	1.575205
150.H	−3.495798	−10.057390	−0.204671
151.H	6.446849	−1.173257	1.522799
152.P	10.559134	2.759648	−0.830675

153.O	12.125375	2.541482	-0.596423
154.O	10.132207	3.333057	-2.140993
155.O	10.005035	1.265207	-0.656224
156.C	10.255728	0.472307	0.572374
157.N	2.947347	-2.070071	-1.966090
158.H	-3.358823	12.643965	-0.516606
159.C	9.820281	-0.967439	0.356414
160.O	8.364963	-1.055568	0.304493
161.C	10.344683	-1.657922	-0.928026
162.C	-3.776573	7.281520	1.328874
163.N	-4.047454	3.644893	1.496112
164.C	-2.670412	3.851733	1.546563
165.H	2.680438	7.626529	-0.784898
166.C	-1.586184	2.927653	1.614022
167.H	-6.941924	8.892831	3.165799
168.H	-7.136944	10.023867	1.805713
169.H	-4.798275	9.871257	2.482082
170.H	-5.378080	7.255053	-0.123027
171.O	-3.552104	7.558916	-1.081745
172.H	-2.768020	7.700950	1.427141
173.H	-5.642214	5.066161	1.362945
174.O	8.064489	7.428869	1.296335
175.H	1.529540	10.160935	1.243051
176.H	2.309535	1.938157	-2.067453
177.H	0.496793	2.956101	1.601080
178.H	1.944639	4.872077	1.581057
179.H	1.174051	6.449618	1.533674
180.P	-2.754024	10.562642	-0.825038
181.O	-2.531443	12.128905	-0.598326
182.O	-3.323825	10.130785	-2.135621
183.N	3.581671	0.331710	1.596406
184.O	-1.262127	10.004888	-0.643710
185.C	-0.467459	10.258932	0.582930
186.C	0.970289	9.818079	0.364332
187.O	1.051873	8.362637	0.310344
188.C	1.659416	10.342134	-0.921501
189.O	3.017282	10.762662	-0.679163
190.C	1.579925	9.146173	-1.907883
191.O	-3.568123	10.080124	0.466784
192.C	9.049572	6.736929	2.097859
193.N	2.823220	5.188598	-1.586003
194.C	9.053567	5.226911	1.883745
195.O	7.772612	4.665136	2.353179
196.C	-4.419550	7.773368	0.022603
197.C	1.637654	7.926115	-0.942769
198.N	0.935523	6.737334	-1.370421
199.C	-0.446592	6.565269	-1.460135
200.C	9.208453	4.768144	0.417941
201.H	-5.510601	9.688451	-0.223519
202.O	10.070994	3.567212	0.463049
203.C	7.765842	4.418329	0.022882
204.C	7.275267	3.777803	1.330643
205.N	-0.769415	5.318247	-1.737816
206.C	4.952986	0.159647	1.616025
207.N	5.447017	-1.095056	1.688094
208.N	5.815225	1.185205	1.591219
209.C	5.214559	2.383083	1.532440
210.H	8.893540	6.943211	3.163517
211.C	0.436122	4.624175	-1.816075
212.C	-5.227251	9.058624	1.884899
213.O	-4.660281	7.779807	2.354313
214.N	5.848489	3.618625	1.449891
215.C	-4.768447	9.216041	0.419429
216.H	10.026786	7.132350	1.804308
217.O	-8.064489	-7.428869	1.296335
218.H	9.864029	4.794085	2.481003
219.C	-9.049572	-6.736929	2.097859
220.C	-9.053567	-5.226911	1.883745
221.O	-7.772612	-4.665136	2.353179
222.H	9.679473	5.509898	-0.226283
223.C	-9.208453	-4.768144	0.417941
224.H	7.246470	5.376073	-0.124629
225.H	3.495798	10.057390	-0.204671
226.O	-10.070994	-3.567212	0.463049
227.C	-4.627363	0.436376	-1.826560
228.C	-3.247179	0.691344	-2.060590
229.O	-2.351634	-0.139469	-2.327449
230.N	-2.947347	2.070071	-1.966090
231.C	-3.884894	3.071454	-1.778795
232.N	-3.454291	4.348542	-1.822102
233.N	-5.190795	2.823206	-1.591767
234.C	-5.490860	1.512018	-1.598334
235.H	-9.680618	-0.924767	1.383272
236.H	-11.323706	-0.507302	0.798607
237.H	-10.166525	1.522684	1.236554
238.H	-11.218710	1.153653	-1.344645
239.O	-9.183652	0.419926	-2.751059
240.H	-9.142359	2.443820	-2.581786
241.H	-7.628622	2.681290	-0.794073
242.H	-7.361729	-1.149448	-1.267998
243.H	-1.940126	2.308896	-2.071777
244.H	-2.450966	4.614050	-1.793023
245.H	-4.120733	5.066385	-1.565172
246.O	10.764007	-3.015975	-0.683426
247.C	9.149188	-1.580277	-1.914940
248.C	7.928698	-1.638455	-0.950039
249.C	3.884894	-3.071454	-1.778795
250.H	11.323706	0.507302	0.798607
251.H	10.166525	-1.522684	1.236554
252.H	10.060809	-3.491071	-0.202415
253.C	4.841032	4.585151	1.427223
254.H	3.358823	-12.643965	-0.516606
255.N	6.739992	-0.935738	-1.377554
256.H	-0.920704	9.688747	1.396859
257.H	11.218710	-1.153653	-1.344645
258.H	-7.266994	7.190537	1.708415
259.H	7.266994	-7.190537	1.708415
260.H	12.632581	3.369774	-0.483659
261.N	-5.848489	-3.618625	1.449891
262.C	-4.585574	4.847119	1.422705
263.H	-7.193636	-7.271831	1.703231
264.H	-12.632581	-3.369774	-0.483659
265.H	-9.454443	-0.345976	-2.202063
266.H	0.346276	-9.452656	-2.192410
267.H	9.454443	0.345976	-2.202063
268.H	-0.346276	9.452656	-2.192410
269.H	8.288909	3.659292	-1.723362
270.H	-3.649282	8.304554	-1.717699
271.H	-8.288909	-3.659292	-1.723362

272.H	3.649282	−8.304554	−1.717699

RNAGQ-Li^+ (Bond Energy: -39445.78) (Symmetry C2)

1.C	6.468190	−1.540348	1.516729
2.N	5.358071	−0.832786	1.599748
3.C	4.323680	−1.763701	1.679325
4.C	2.909472	−1.589277	1.727795
5.O	2.266251	−0.517514	1.745326
6.N	2.227321	−2.827604	1.746256
7.C	2.838601	−4.066870	1.771349
8.N	2.059028	−5.167229	1.836904
9.N	4.168965	−4.222952	1.746454
10.C	4.839215	−3.063433	1.671509
11.H	10.660469	−3.723944	3.266130
12.H	11.452062	−4.468337	1.856551
13.H	9.408148	−5.672300	2.451155
14.H	9.928648	−4.936639	−0.211320
15.H	8.445670	−3.024411	−0.020423
16.O	7.106560	−4.258069	−1.037111
17.H	6.526361	−4.922600	1.440671
18.H	7.468829	−1.140005	1.435089
19.H	1.187848	−2.756443	1.736514
20.H	1.030671	−5.148332	1.719748
21.H	2.538284	−6.047887	1.679561
22.P	8.206470	−7.174396	−0.997847
23.O	8.950083	−8.582754	−0.866583
24.O	8.438460	−6.386366	−2.244595
25.O	6.671899	−7.617978	−0.882017
26.C	6.160252	−8.416639	0.258220
27.C	−2.994969	−1.064518	−1.529078
28.C	4.708440	−8.782113	0.005181
29.O	3.872117	−7.590327	0.105856
30.C	4.397135	−9.427170	−1.371911
31.O	3.506122	−10.554639	−1.259071
32.C	3.782239	−8.266783	−2.198401
33.C	3.075082	−7.434617	−1.092206
34.C	−4.323680	1.763701	1.679325
35.N	2.938192	−6.017038	−1.346335
36.C	−2.909472	1.589277	1.727795
37.H	−4.632134	2.519569	−1.573205
38.N	−3.576011	0.210912	−1.536566
39.N	−5.163477	−2.055435	1.840601
40.H	−6.305622	1.963227	−1.569763
41.C	−4.939833	0.466065	−1.561793
42.O	−7.522719	−4.753722	−2.948928
43.O	−1.738739	−1.194810	−1.524911
44.H	−8.637391	−3.051648	−2.923974
45.C	7.944479	−3.997686	0.080309
46.N	−2.908971	−6.215069	1.569514
47.H	−5.317552	−4.995396	−1.192779
48.H	−9.326270	−6.777321	0.324252
49.H	−9.809276	−5.297584	−1.882511
50.O	−7.106560	4.258069	−1.037111
51.C	3.953839	−5.064142	−1.336696
52.N	3.479675	−3.840113	−1.443156
53.O	−0.513965	−2.262110	1.740241
54.C	−4.063159	−2.835160	1.775406
55.C	−3.913219	−10.576079	2.202097
56.N	−2.824143	−2.223648	1.747880
57.C	7.135918	−4.012461	1.388014
58.C	−5.328357	−1.738448	−1.457209
59.O	−2.266251	0.517514	1.745326
60.H	−9.985035	2.038935	1.910137
61.N	−5.358071	0.832786	1.599748
62.N	−4.219095	−4.165643	1.754034
63.C	−3.059416	−4.835931	1.680754
64.N	−5.321836	1.746935	−1.669660
65.O	2.656972	10.616098	1.486419
66.C	3.913219	10.576079	2.202097
67.C	4.727363	9.318612	1.917725
68.O	3.992584	8.143712	2.423310
69.C	5.007639	9.040513	0.424993
70.O	6.395691	8.537354	0.357810
71.C	3.986393	7.942926	0.088434
72.C	4.007436	7.132763	1.395051
73.N	2.908971	6.215069	1.569514
74.C	1.536027	6.464538	1.525729
75.N	0.828761	5.354048	1.606150
76.C	1.759885	4.319910	1.686023
77.C	1.585793	2.905466	1.728724
78.O	0.513965	2.262110	1.740241
79.N	2.824143	2.223648	1.747880
80.C	4.063159	2.835160	1.775406
81.N	5.163477	2.055435	1.840601
82.N	4.219095	4.165643	1.754034
83.C	3.059416	4.835931	1.680754
84.H	3.743892	10.653101	3.282848
85.H	4.489303	11.446826	1.874700
86.H	5.681191	9.391298	2.452171
87.H	4.927781	9.925935	−0.205075
88.H	3.013582	8.446645	−0.004468
89.O	4.236375	7.106068	−1.031970
90.H	4.917919	6.523309	1.443596
91.H	1.135431	7.465184	1.445354
92.H	2.753647	1.184057	1.738763
93.H	5.145805	1.027571	1.720091
94.H	6.044740	2.535249	1.689052
95.P	7.158790	8.206066	−1.011855
96.O	8.561364	8.962874	−0.895026
97.O	6.358577	8.429952	−2.252471
98.O	7.615785	6.675856	−0.896372
99.C	8.422047	6.170702	0.241203
100.C	8.790051	4.718874	−0.007739
101.O	7.600405	3.880309	0.103043
102.C	9.428246	4.402672	−1.386971
103.O	10.557814	3.513788	−1.276949
104.C	8.264373	3.782471	−2.204485
105.C	7.439103	3.078381	−1.090922
106.N	6.020203	2.939215	−1.338373
107.C	5.066690	3.954241	−1.326637
108.N	3.842997	3.479538	−1.433707
109.C	3.972230	2.094763	−1.510757
110.C	2.994969	1.064518	−1.529078
111.O	1.738739	1.194810	−1.524911
112.N	3.576011	−0.210912	−1.536566

113.C	4.939833	−0.466065	−1.561793
114.N	5.321836	−1.746935	−1.669660
115.N	5.860047	0.507896	−1.503074
116.C	5.328357	1.738448	−1.457209
117.H	7.818776	6.261853	1.147283
118.H	9.326270	6.777321	0.324252
119.H	9.489931	4.437742	0.788781
120.H	9.809276	5.297584	−1.882511
121.O	7.522719	4.753722	−2.948928
122.H	8.637391	3.051648	−2.923974
123.H	7.824693	2.064618	−0.927270
124.H	5.317552	4.995396	−1.192779
125.H	2.885189	−0.984365	−1.536501
126.H	4.632134	−2.519569	−1.573205
127.H	6.305622	−1.963227	−1.569763
128.O	−4.757625	7.530705	−2.943516
129.H	−3.053568	8.642804	−2.918606
130.O	−2.656972	−10.616098	1.486419
131.H	−2.060046	7.818200	−0.930877
132.H	−4.995115	5.315496	−1.204421
133.H	0.984669	2.881189	−1.531414
134.H	2.520466	4.627472	−1.563848
135.H	1.965949	6.300669	−1.564046
136.H	−6.526361	4.922600	1.440671
137.H	−7.468829	1.140005	1.435089
138.H	2.729346	−10.304028	−0.724803
139.H	−1.187848	2.756443	1.736514
140.C	−3.953839	5.064142	−1.336696
141.N	−3.479675	3.840113	−1.443156
142.C	−2.094421	3.968672	−1.516645
143.C	−1.064224	2.991457	−1.531162
144.O	−1.195150	1.735101	−1.527511
145.N	1.748081	5.317096	−1.662757
146.N	−0.507097	5.856244	−1.503983
147.C	−1.737645	5.324597	−1.462120
148.H	−6.249502	7.808282	1.161035
149.H	−1.030671	5.148332	1.719748
150.H	10.314140	2.742683	−0.731359
151.H	−2.538284	6.047887	1.679561
152.P	−8.206470	7.174396	−0.997847
153.O	−8.950083	8.582754	−0.866583
154.O	−8.438460	6.386366	−2.244595
155.O	−6.671899	7.617978	−0.882017
156.C	−6.160252	8.416639	0.258220
157.N	0.211190	3.571989	−1.533810
158.H	−8.486312	−9.932293	−0.788546
159.C	−4.708440	8.782113	0.005181
160.O	−3.872117	7.590327	0.105856
161.C	−4.397135	9.427170	−1.371911
162.C	−4.007436	−7.132763	1.395051
163.N	−0.828761	−5.354048	1.606150
164.C	−1.759885	−4.319910	1.686023
165.H	−7.824693	−2.064618	−0.927270
166.C	−1.585793	−2.905466	1.728724
167.H	−3.743892	−10.653101	3.282848
168.H	−4.489303	−11.446826	1.874700
169.H	−5.681191	−9.391298	2.452171
170.H	−3.013582	−8.446645	−0.004468
171.O	−4.236375	−7.106068	−1.031970
172.H	−4.917919	−6.523309	1.443596
173.H	−1.135431	−7.465184	1.445354
174.O	−10.606324	2.643497	1.466070
175.H	−9.489931	−4.437742	0.788781
176.H	−2.885189	0.984365	−1.536501
177.H	−2.753647	−1.184057	1.738763
178.H	−5.145805	−1.027571	1.720091
179.H	−6.044740	−2.535249	1.689052
180.P	−7.158790	−8.206066	−1.011855
181.O	−8.561364	−8.962874	−0.895026
182.O	−6.358577	−8.429952	−2.252471
183.N	−2.227321	2.827604	1.746256
184.O	−7.615785	−6.675856	−0.896372
185.C	−8.422047	−6.170702	0.241203
186.C	−8.790051	−4.718874	−0.007739
187.O	−7.600405	−3.880309	0.103043
188.C	−9.428246	−4.402672	−1.386971
189.O	−10.557814	−3.513788	−1.276949
190.C	−8.264373	−3.782471	−2.204485
191.O	−6.395691	−8.537354	0.357810
192.C	−10.578862	3.897493	2.186398
193.N	−5.860047	−0.507896	−1.503074
194.C	−9.326104	4.722215	1.911270
195.O	−8.147192	3.993156	2.416105
196.C	−3.986393	−7.942926	0.088434
197.C	−7.439103	−3.078381	−1.090922
198.N	−6.020203	−2.939215	−1.338373
199.C	−5.066690	−3.954241	−1.326637
200.C	−9.045169	5.013986	0.421708
201.H	−4.927781	−9.925935	−0.205075
202.O	−8.545494	6.404154	0.366072
203.C	−7.944479	3.997686	0.080309
204.C	−7.135918	4.012461	1.388014
205.N	−3.842997	−3.479538	−1.433707
206.C	−2.838601	4.066870	1.771349
207.N	−2.059028	5.167229	1.836904
208.N	−4.168965	4.222952	1.746454
209.C	−4.839215	3.063433	1.671509
210.H	−10.660469	3.723944	3.266130
211.C	−3.972230	−2.094763	−1.510757
212.C	−4.727363	−9.318612	1.917725
213.O	−3.992584	−8.143712	2.423310
214.N	−6.218242	2.913311	1.558808
215.C	−5.007639	−9.040513	0.424993
216.H	−11.452062	4.468337	1.856551
217.O	10.606324	−2.643497	1.466070
218.H	−9.408148	5.672300	2.451155
219.C	10.578862	−3.897493	2.186398
220.C	9.326104	−4.722215	1.911270
221.O	8.147192	−3.993156	2.416105
222.H	−9.928648	4.936639	−0.211320
223.C	9.045169	−5.013986	0.421708
224.H	−8.445670	3.024411	−0.020423
225.H	−10.314140	−2.742683	−0.731359
226.O	8.545494	−6.404154	0.366072
227.C	2.094421	−3.968672	−1.516645
228.C	1.064224	−2.991457	−1.531162
229.O	1.195150	−1.735101	−1.527511
230.N	−0.211190	−3.571989	−1.533810
231.C	−0.466819	−4.935777	−1.559146

232.N	−1.748081	−5.317096	−1.662757
233.N	0.507097	−5.856244	−1.503983
234.C	1.737645	−5.324597	−1.462120
235.H	6.249502	−7.808282	1.161035
236.H	6.763687	−9.322464	0.349098
237.H	4.422193	−9.477493	0.803527
238.H	5.293510	−9.812785	−1.861216
239.O	4.757625	−7.530705	−2.943516
240.H	3.053568	−8.642804	−2.918606
241.H	2.060046	−7.818200	−0.930877
242.H	4.995115	−5.315496	−1.204421
243.H	−0.984669	−2.881189	−1.531414
244.H	−2.520466	−4.627472	−1.563848
245.H	−1.965949	−6.300669	−1.564046
246.O	−3.506122	10.554639	−1.259071
247.C	−3.782239	8.266783	−2.198401
248.C	−3.075082	7.434617	−1.092206
249.C	0.466819	4.935777	−1.559146
250.H	−6.763687	9.322464	0.349098
251.H	−4.422193	9.477493	0.803527
252.H	−2.729346	10.304028	−0.724803
253.C	−6.468190	1.540348	1.516729
254.H	8.486312	9.932293	−0.788546
255.N	−2.938192	6.017038	−1.346335
256.H	−7.818776	−6.261853	1.147283
257.H	−5.293510	9.812785	−1.861216
258.H	−2.051786	−9.991910	1.925730
259.H	2.051786	9.991910	1.925730
260.H	−9.915566	8.516848	−0.727171
261.N	6.218242	−2.913311	1.558808
262.C	−1.536027	−6.464538	1.525729
263.H	9.985035	−2.038935	1.910137
264.H	9.915566	−8.516848	−0.727171
265.H	5.555587	−7.424255	−2.383382
266.H	7.419104	5.554169	−2.391951
267.H	−5.555587	7.424255	−2.383382
268.H	−7.419104	−5.554169	−2.391951
269.H	−7.618794	4.761855	−1.711368
270.H	−4.738610	−7.617483	−1.708084
271.H	7.618794	−4.761855	−1.711368
272.H	4.738610	7.617483	−1.708084
273.Li	0.000000	0.000000	−1.283936

$_{RNA}$GQ-Na^{+} (Bond Energy: -39436.46) (Symmetry C2)

1.C	6.411738	−1.501935	1.472657
2.N	5.290931	−0.808173	1.495800
3.C	4.264853	−1.748217	1.579240
4.C	2.849378	−1.600381	1.539141
5.O	2.187238	−0.537401	1.445160
6.N	2.186598	−2.842795	1.596870
7.C	2.813848	−4.072830	1.690539
8.N	2.048125	−5.178777	1.759850
9.N	4.146157	−4.206621	1.720761
10.C	4.800021	−3.040820	1.634726
11.H	10.628294	−3.645073	3.288790
12.H	11.423709	−4.421511	1.898753
13.H	9.372868	−5.605815	2.503692
14.H	9.902864	−4.913653	−0.170945
15.H	8.420226	−2.994932	−0.004169
16.O	7.085903	−4.238577	−1.013806
17.H	6.507245	−4.883002	1.478530
18.H	7.408940	−1.089654	1.409693
19.H	1.148790	−2.781806	1.545247
20.H	1.020841	−5.164097	1.620784
21.H	2.540596	−6.059425	1.649176
22.P	8.172975	−7.158557	−0.925836
23.O	8.913193	−8.567010	−0.775765
24.O	8.406353	−6.388992	−2.184045
25.O	6.636775	−7.596827	−0.803688
26.C	6.124542	−8.373494	0.351993
27.C	−3.036993	−1.124254	−1.591357
28.C	4.687776	−8.790879	0.091281
29.O	3.808894	−7.626762	0.142386
30.C	4.411037	−9.491442	−1.264069
31.O	3.529186	−10.623310	−1.122321
32.C	3.797059	−8.373291	−2.147454
33.C	3.059658	−7.501238	−1.091276
34.C	−4.264853	1.748217	1.579240
35.N	2.945466	−6.090746	−1.394301
36.C	−2.849378	1.600381	1.539141
37.H	−4.624499	2.507086	−1.635801
38.N	−3.593423	0.165471	−1.612143
39.N	−5.178336	−2.048502	1.762990
40.H	−6.290959	1.963851	−1.633127
41.C	−4.950440	0.444618	−1.639315
42.O	−7.660440	−4.778886	−2.912124
43.O	−1.788503	−1.277111	−1.545839
44.H	−8.787900	−3.087809	−2.863584
45.C	7.919074	−3.967579	0.103765
46.N	−2.872994	−6.178112	1.554000
47.H	−5.414042	−5.009766	−1.221689
48.H	−9.257992	−6.746289	0.489730
49.H	−9.885835	−5.320922	−1.718364
50.O	−7.085903	4.238577	−1.013806
51.C	3.974919	−5.149914	−1.373971
52.N	3.520936	−3.920080	−1.498362
53.O	−0.536641	−2.185583	1.446339
54.C	−4.071839	−2.813616	1.692676
55.C	−3.847384	−10.549629	2.222906
56.N	−2.842120	−2.185675	1.599272
57.C	7.108578	−3.968523	1.410567
58.C	−5.380659	−1.755924	−1.535554
59.O	−2.187238	0.537401	1.445160
60.H	−9.964606	1.986186	1.892260
61.N	−5.290931	0.808173	1.495800
62.N	−4.205115	−4.145978	1.721436
63.C	−3.039052	−4.799284	1.634007
64.N	−5.311079	1.734826	−1.746202
65.O	2.605733	10.591180	1.482472
66.C	3.847384	10.549629	2.222906
67.C	4.666318	9.292146	1.953049
68.O	3.918230	8.116345	2.438432
69.C	4.980545	9.017394	0.466256
70.O	6.369942	8.512529	0.430429
71.C	3.967401	7.920622	0.104726

72.C	3.965998	7.107709	1.409910
73.N	2.872994	6.178112	1.554000
74.C	1.499754	6.410065	1.466257
75.N	0.806507	5.289045	1.491379
76.C	1.746778	4.263543	1.578389
77.C	1.599383	2.848024	1.540229
78.O	0.536641	2.185583	1.446339
79.N	2.842120	2.185675	1.599272
80.C	4.071839	2.813616	1.692676
81.N	5.178336	2.048502	1.762990
82.N	4.205115	4.145978	1.721436
83.C	3.039052	4.799284	1.634007
84.H	3.656819	10.625441	3.300257
85.H	4.430450	11.420342	1.908125
86.H	5.608005	9.361644	2.508817
87.H	4.916773	9.904315	-0.163662
88.H	2.995645	8.423503	-0.003868
89.O	4.238958	7.088449	-1.013386
90.H	4.880488	6.506391	1.478207
91.H	1.087012	7.406812	1.399331
92.H	2.781689	1.147745	1.548751
93.H	5.164447	1.021331	1.623578
94.H	6.058372	2.541621	1.650207
95.P	7.160439	8.171245	-0.920831
96.O	8.567931	8.912807	-0.768191
97.O	6.393798	8.405456	-2.180517
98.O	7.598337	6.634757	-0.799431
99.C	8.373360	6.120044	0.356425
100.C	8.790641	4.683594	0.092550
101.O	7.627383	3.803752	0.141906
102.C	9.490559	4.410552	-1.263844
103.O	10.621942	3.527213	-1.124980
104.C	8.371965	3.799720	-2.148965
105.C	7.499978	3.059229	-1.094896
106.N	6.089213	2.945877	-1.396119
107.C	5.148246	3.975223	-1.374811
108.N	3.918256	3.521026	-1.496653
109.C	4.032725	2.135564	-1.593874
110.C	3.036993	1.124254	-1.591357
111.O	1.788503	1.277111	-1.545839
112.N	3.593423	-0.165471	-1.612143
113.C	4.950440	-0.444618	-1.639315
114.N	5.311079	-1.734826	-1.746202
115.N	5.889057	0.513147	-1.580468
116.C	5.380659	1.755924	-1.535554
117.H	7.732261	6.174520	1.239146
118.H	9.257992	6.746289	0.489730
119.H	9.466753	4.408799	0.911353
120.H	9.885835	5.320922	-1.718364
121.O	7.660440	4.778886	-2.912124
122.H	8.787900	3.087809	-2.863584
123.H	7.868573	2.035243	-0.960224
124.H	5.414042	5.009766	-1.221689
125.H	2.893324	-0.933036	-1.599514
126.H	4.624499	-2.507086	-1.635801
127.H	6.290959	-1.963851	-1.633127
128.O	-4.774501	7.661274	-2.912448
129.H	-3.083440	8.789118	-2.860618
130.O	-2.605733	-10.591180	1.482472
131.H	-2.036280	7.869965	-0.952346
132.H	-5.009237	5.415536	-1.219141
133.H	0.932431	2.894430	-1.601542
134.H	2.507058	4.625800	-1.635963
135.H	1.963939	6.292643	-1.633822
136.H	-6.507245	4.883002	1.478530
137.H	-7.408940	1.089654	1.409693
138.H	2.742807	-10.360525	-0.608397
139.H	-1.148790	2.781806	1.545247
140.C	-3.974919	5.149914	-1.373971
141.N	-3.520936	3.920080	-1.498362
142.C	-2.135598	4.034785	-1.597030
143.C	-1.124587	3.038880	-1.595904
144.O	-1.278060	1.790492	-1.551790
145.N	1.735066	5.312669	-1.746603
146.N	-0.512767	5.890679	-1.581237
147.C	-1.755698	5.382518	-1.536462
148.H	-6.181007	7.733636	1.235515
149.H	-1.020841	5.164097	1.620784
150.H	10.356661	2.735316	-0.620797
151.H	-2.540596	6.059425	1.649176
152.P	-8.172975	7.158557	-0.925836
153.O	-8.913193	8.567010	-0.775765
154.O	-8.406353	6.388992	-2.184045
155.O	-6.636775	7.596827	-0.803688
156.C	-6.124542	8.373494	0.351993
157.N	0.165363	3.594927	-1.615930
158.H	-8.499694	-9.879667	-0.637192
159.C	-4.687776	8.790879	0.091281
160.O	-3.808894	7.626762	0.142386
161.C	-4.411037	9.491442	-1.264069
162.C	-3.965998	-7.107709	1.409910
163.N	-0.806507	-5.289045	1.491379
164.C	-1.746778	-4.263543	1.578389
165.H	-7.868573	-2.035243	-0.960224
166.C	-1.599383	-2.848024	1.540229
167.H	-3.656819	-10.625441	3.300257
168.H	-4.430450	-11.420342	1.908125
169.H	-5.608005	-9.361644	2.508817
170.H	-2.995645	-8.423503	-0.003868
171.O	-4.238958	-7.088449	-1.013386
172.H	-4.880488	-6.506391	1.478207
173.H	-1.087012	-7.406812	1.399331
174.O	-10.588725	2.601257	1.466928
175.H	-9.466753	-4.408799	0.911353
176.H	-2.893324	0.933036	-1.599514
177.H	-2.781689	-1.147745	1.548751
178.H	-5.164447	-1.021331	1.623578
179.H	-6.058372	-2.541621	1.650207
180.P	-7.160439	-8.171245	-0.920831
181.O	-8.567931	-8.912807	-0.768191
182.O	-6.393798	-8.405456	-2.180517
183.N	-2.186598	2.842795	1.596870
184.O	-7.598337	-6.634757	-0.799431
185.C	-8.373360	-6.120044	0.356425
186.C	-8.790641	-4.683594	0.092550
187.O	-7.627383	-3.803752	0.141906
188.C	-9.490559	-4.410552	-1.263844
189.O	-10.621942	-3.527213	-1.124980
190.C	-8.371965	-3.799720	-2.148965

191.O	-6.369942	-8.512529	0.430429
192.C	-10.551529	3.840060	2.212335
193.N	-5.889057	-0.513147	-1.580468
194.C	-9.296598	4.664680	1.947467
195.O	-8.118900	3.922111	2.437372
196.C	-3.967401	-7.920622	0.104726
197.C	-7.499978	-3.059229	-1.094896
198.N	-6.089213	-2.945877	-1.396119
199.C	-5.148246	-3.975223	-1.374811
200.C	-9.018205	4.979331	0.461713
201.H	-4.916773	-9.904315	-0.163662
202.O	-8.515307	6.369828	0.426421
203.C	-7.919074	3.967579	0.103765
204.C	-7.108578	3.968523	1.410567
205.N	-3.918256	-3.521026	-1.496653
206.C	-2.813848	4.072830	1.690539
207.N	-2.048125	5.178777	1.759850
208.N	-4.146157	4.206621	1.720761
209.C	-4.800021	3.040820	1.634726
210.H	-10.628294	3.645073	3.288790
211.C	-4.032725	-2.135564	-1.593874
212.C	-4.666318	-9.292146	1.953049
213.O	-3.918230	-8.116345	2.438432
214.N	-6.179174	2.875315	1.557938
215.C	-4.980545	-9.017394	0.466256
216.H	-11.423709	4.421511	1.898753
217.O	10.588725	-2.601257	1.466928
218.H	-9.372868	5.605815	2.503692
219.C	10.551529	-3.840060	2.212335
220.C	9.296598	-4.664680	1.947467
221.O	8.118900	-3.922111	2.437372
222.H	-9.902864	4.913653	-0.170945
223.C	9.018205	-4.979331	0.461713
224.H	-8.420226	2.994932	-0.004169
225.H	-10.356661	-2.735316	-0.620797
226.O	8.515307	-6.369828	0.426421
227.C	2.135598	-4.034785	-1.597030
228.C	1.124587	-3.038880	-1.595904
229.O	1.278060	-1.790492	-1.551790
230.N	-0.165363	-3.594927	-1.615930
231.C	-0.444725	-4.952009	-1.641069
232.N	-1.735066	-5.312669	-1.746603
233.N	0.512767	-5.890679	-1.581237
234.C	1.755698	-5.382518	-1.536462
235.H	6.181007	-7.733636	1.235515
236.H	6.751362	-9.258178	0.483234
237.H	4.414462	-9.466309	0.910956
238.H	5.320188	-9.885758	-1.721965
239.O	4.774501	-7.661274	-2.912448
240.H	3.083440	-8.789118	-2.860618
241.H	2.036280	-7.869965	-0.952346
242.H	5.009237	-5.415536	-1.219141
243.H	-0.932431	-2.894430	-1.601542
244.H	-2.507058	-4.625800	-1.635963
245.H	-1.963939	-6.292643	-1.633822
246.O	-3.529186	10.623310	-1.122321
247.C	-3.797059	8.373291	-2.147454
248.C	-3.059658	7.501238	-1.091276
249.C	0.444725	4.952009	-1.641069
250.H	-6.751362	9.258178	0.483234
251.H	-4.414462	9.466309	0.910956
252.H	-2.742807	10.360525	-0.608397
253.C	-6.411738	1.501935	1.472657
254.H	8.499694	9.879667	-0.637192
255.N	-2.945466	6.090746	-1.394301
256.H	-7.732261	-6.174520	1.239146
257.H	-5.320188	9.885758	-1.721965
258.H	-1.992595	-9.964608	1.907174
259.H	1.992595	9.964608	1.907174
260.H	-9.881264	8.501334	-0.655026
261.N	6.179174	-2.875315	1.557938
262.C	-1.499754	-6.410065	1.466257
263.H	9.964606	-1.986186	1.892260
264.H	9.881264	-8.501334	-0.655026
265.H	5.561861	-7.516447	-2.346303
266.H	7.515684	5.564934	-2.344233
267.H	-5.561861	7.516447	-2.346303
268.H	-7.515684	-5.564934	-2.344233
269.H	-7.597801	4.757805	-1.676713
270.H	-4.754501	-7.602038	-1.677611
271.H	7.597801	-4.757805	-1.676713
272.H	4.754501	7.602038	-1.677611
273.Na	0.000000	0.000000	-0.265516

$_{RNA}$GQ-K^{+} (Bond Energy: -39439.14) (Symmetry C2)

1.C	6.439278	-1.552577	1.524094
2.N	5.325555	-0.849201	1.582529
3.C	4.293612	-1.785012	1.641441
4.C	2.881221	-1.623288	1.640036
5.O	2.228363	-0.549997	1.609396
6.N	2.204123	-2.859721	1.655240
7.C	2.819682	-4.099178	1.699727
8.N	2.041155	-5.197165	1.752675
9.N	4.150698	-4.246025	1.699112
10.C	4.816355	-3.084198	1.644090
11.H	10.626327	-3.748879	3.316812
12.H	11.429371	-4.490640	1.912367
13.H	9.372763	-5.687149	2.481217
14.H	9.927200	-4.947553	-0.173521
15.H	8.449291	-3.028319	0.013173
16.O	7.118479	-4.247603	-1.030096
17.H	6.513516	-4.934634	1.442213
18.H	7.439962	-1.147932	1.466567
19.H	1.166690	-2.795288	1.645923
20.H	1.011759	-5.174228	1.643361
21.H	2.521577	-6.082507	1.630628
22.P	8.210934	-7.185964	-0.977763
23.O	8.982387	-8.579537	-0.850734
24.O	8.427771	-6.391509	-2.223332
25.O	6.684755	-7.657755	-0.860667
26.C	6.188445	-8.447471	0.293162
27.C	-3.070247	-1.182416	-1.693353
28.C	4.740264	-8.838145	0.055833
29.O	3.886666	-7.656565	0.127370
30.C	4.428921	-9.526732	-1.299074
31.O	3.539935	-10.651471	-1.147996
32.C	3.809850	-8.395594	-2.161374

33.C	3.102220	−7.526038	−1.082798
34.C	−4.293612	1.785012	1.641441
35.N	2.983966	−6.115167	−1.379180
36.C	−2.881221	1.623288	1.640036
37.H	−4.642316	2.473977	−1.634186
38.N	−3.616640	0.114598	−1.671248
39.N	−5.196667	−2.045259	1.785385
40.H	−6.304357	1.928932	−1.553835
41.C	−4.971352	0.403341	−1.618401
42.O	−7.710699	−4.758542	−2.910193
43.O	−1.824204	−1.343882	−1.741945
44.H	−8.811996	−3.051617	−2.809972
45.C	7.943074	−4.000673	0.099344
46.N	−2.925949	−6.196562	1.523709
47.H	−5.449215	−5.054373	−1.227085
48.H	−9.349572	−6.815033	0.406487
49.H	−9.943847	−5.304209	−1.738421
50.O	−7.118479	4.247603	−1.030096
51.C	4.017916	−5.178477	−1.394903
52.N	3.569360	−3.950431	−1.554780
53.O	−0.550606	−2.229850	1.604738
54.C	−4.098843	−2.822965	1.715022
55.C	−3.890593	−10.562776	2.178865
56.N	−2.859951	−2.206201	1.668369
57.C	7.120364	−4.022212	1.398519
58.C	−5.410667	−1.797104	−1.503803
59.O	−2.228363	0.549997	1.609396
60.H	−9.973673	2.054548	1.961268
61.N	−5.325555	0.849201	1.582529
62.N	−4.245306	−4.153976	1.700678
63.C	−3.083839	−4.818676	1.626557
64.N	−5.328605	1.697347	−1.692751
65.O	2.639750	10.593197	1.453805
66.C	3.890593	10.562776	2.178865
67.C	4.717767	9.312097	1.900586
68.O	3.987856	8.129208	2.395476
69.C	5.017880	9.038777	0.410839
70.O	6.408048	8.538432	0.362623
71.C	4.004179	7.938884	0.059734
72.C	4.019923	7.123171	1.363436
73.N	2.925949	6.196562	1.523709
74.C	1.551990	6.438566	1.472333
75.N	0.849014	5.325085	1.538211
76.C	1.785135	4.295014	1.619217
77.C	1.623723	2.882866	1.635441
78.O	0.550606	2.229850	1.604738
79.N	2.859951	2.206201	1.668369
80.C	4.098843	2.822965	1.715022
81.N	5.196667	2.045259	1.785385
82.N	4.245306	4.153976	1.700678
83.C	3.083839	4.818676	1.626557
84.H	3.713034	10.638375	3.258425
85.H	4.462152	11.438094	1.855666
86.H	5.665210	9.391398	2.445383
87.H	4.944086	9.925352	−0.218481
88.H	3.030078	8.439740	−0.036093
89.O	4.263043	7.110408	−1.064079
90.H	4.933883	6.519526	1.417809
91.H	1.147412	7.438044	1.397647
92.H	2.795806	1.168745	1.664727
93.H	5.174770	1.015422	1.682015
94.H	6.082751	2.524556	1.664181
95.P	7.197588	8.210924	−0.992553
96.O	8.587687	8.987752	−0.859853
97.O	6.414566	8.415503	−2.247368
98.O	7.672953	6.687309	−0.858337
99.C	8.451292	6.201593	0.307163
100.C	8.835079	4.748075	0.091501
101.O	7.647245	3.903320	0.161553
102.C	9.534930	4.416070	−1.252976
103.O	10.653647	3.523242	−1.080434
104.C	8.408538	3.792583	−2.118182
105.C	7.525780	3.102886	−1.038852
106.N	6.117593	2.985326	−1.348101
107.C	5.182503	4.020386	−1.380951
108.N	3.955506	3.572237	−1.550352
109.C	4.069731	2.185235	−1.625527
110.C	3.070247	1.182416	−1.693353
111.O	1.824204	1.343882	−1.741945
112.N	3.616640	−0.114598	−1.671248
113.C	4.971352	−0.403341	−1.618401
114.N	5.328605	−1.697347	−1.692751
115.N	5.911769	0.549352	−1.516207
116.C	5.410667	1.797104	−1.503803
117.H	7.823270	6.302414	1.195121
118.H	9.349572	6.815033	0.406487
119.H	9.501201	4.482161	0.921565
120.H	9.943847	5.304209	−1.738421
121.O	7.710699	4.758542	−2.910193
122.H	8.811996	3.051617	−2.809972
123.H	7.889005	2.084003	−0.857080
124.H	5.449215	5.054373	−1.227085
125.H	2.918919	−0.882886	−1.714825
126.H	4.642316	−2.473977	−1.634186
127.H	6.304357	−1.928932	−1.553835
128.O	−4.781492	7.686043	−2.935859
129.H	−3.079273	8.796459	−2.865607
130.O	−2.639750	−10.593197	1.453805
131.H	−2.082228	7.894745	−0.918754
132.H	−5.051007	5.445603	−1.235492
133.H	0.885771	2.916148	−1.728249
134.H	2.476013	4.642642	−1.656628
135.H	1.927676	6.303793	−1.599867
136.H	−6.513516	4.934634	1.442213
137.H	−7.439962	1.147932	1.466567
138.H	2.763933	−10.384218	−0.620774
139.H	−1.166690	2.795288	1.645923
140.C	−4.017916	5.178477	−1.394903
141.N	−3.569360	3.950431	−1.554780
142.C	−2.183119	4.065290	−1.640288
143.C	−1.179974	3.065955	−1.706849
144.O	−1.341105	1.819574	−1.749757
145.N	1.698513	5.326460	−1.732170
146.N	−0.548429	5.909640	−1.557838
147.C	−1.795771	5.407817	−1.534556
148.H	−6.273795	7.824833	1.186532
149.H	−1.011759	5.174228	1.643361
150.H	10.374732	2.748742	−0.556936
151.H	−2.521577	6.082507	1.630628

152.P	−8.210934	7.185964	−0.977763
153.O	−8.982387	8.579537	−0.850734
154.O	−8.427771	6.391509	−2.223332
155.O	−6.684755	7.657755	−0.860667
156.C	−6.188445	8.447471	0.293162
157.N	0.116669	3.613556	−1.691203
158.H	−8.497858	−9.954930	−0.745564
159.C	−4.740264	8.838145	0.055833
160.O	−3.886666	7.656565	0.127370
161.C	−4.428921	9.526732	−1.299074
162.C	−4.019923	−7.123171	1.363436
163.N	−0.849014	−5.325085	1.538211
164.C	−1.785135	−4.295014	1.619217
165.H	−7.889005	−2.084003	−0.857080
166.C	−1.623723	−2.882866	1.635441
167.H	−3.713034	−10.638375	3.258425
168.H	−4.462152	−11.438094	1.855666
169.H	−5.665210	−9.391398	2.445383
170.H	−3.030078	−8.439740	−0.036093
171.O	−4.263043	−7.110408	−1.064079
172.H	−4.933883	−6.519526	1.417809
173.H	−1.147412	−7.438044	1.397647
174.O	−10.596124	2.660569	1.520803
175.H	−9.501201	−4.482161	0.921565
176.H	−2.918919	0.882886	−1.714825
177.H	−2.795806	−1.168745	1.664727
178.H	−5.174770	−1.015422	1.682015
179.H	−6.082751	−2.524556	1.664181
180.P	−7.197588	−8.210924	−0.992553
181.O	−8.587687	−8.987752	−0.859853
182.O	−6.414566	−8.415503	−2.247368
183.N	−2.204123	2.859721	1.655240
184.O	−7.672953	−6.687309	−0.858337
185.C	−8.451292	−6.201593	0.307163
186.C	−8.835079	−4.748075	0.091501
187.O	−7.647245	−3.903320	0.161553
188.C	−9.534930	−4.416070	−1.252976
189.O	−10.653647	−3.523242	−1.080434
190.C	−8.408538	−3.792583	−2.118182
191.O	−6.408048	−8.538432	0.362623
192.C	−10.555391	3.916987	2.235443
193.N	−5.911769	−0.549352	−1.516207
194.C	−9.301881	4.734916	1.943413
195.O	−8.120312	4.001692	2.436589
196.C	−4.004179	−7.938884	0.059734
197.C	−7.525780	−3.102886	−1.038852
198.N	−6.117593	−2.985326	−1.348101
199.C	−5.182503	−4.020386	−1.380951
200.C	−9.036302	5.022025	0.449535
201.H	−4.944086	−9.925352	−0.218481
202.O	−8.530505	6.409645	0.387117
203.C	−7.943074	4.000673	0.099344
204.C	−7.120364	4.022212	1.398519
205.N	−3.955506	−3.572237	−1.550352
206.C	−2.819682	4.099178	1.699727
207.N	−2.041155	5.197165	1.752675
208.N	−4.150698	4.246025	1.699112
209.C	−4.816355	3.084198	1.644090
210.H	−10.626327	3.748879	3.316812
211.C	−4.069731	−2.185235	−1.625527
212.C	−4.717767	−9.312097	1.900586
213.O	−3.987856	−8.129208	2.395476
214.N	−6.195533	2.926863	1.560576
215.C	−5.017880	−9.038777	0.410839
216.H	−11.429371	4.490640	1.912367
217.O	10.596124	−2.660569	1.520803
218.H	−9.372763	5.687149	2.481217
219.C	10.555391	−3.916987	2.235443
220.C	9.301881	−4.734916	1.943413
221.O	8.120312	−4.001692	2.436589
222.H	−9.927200	4.947553	−0.173521
223.C	9.036302	−5.022025	0.449535
224.H	−8.449291	3.028319	0.013173
225.H	−10.374732	−2.748742	−0.556936
226.O	8.530505	−6.409645	0.387117
227.C	2.183119	−4.065290	−1.640288
228.C	1.179974	−3.065955	−1.706849
229.O	1.341105	−1.819574	−1.749757
230.N	−0.116669	−3.613556	−1.691203
231.C	−0.404532	−4.968684	−1.652336
232.N	−1.698513	−5.326460	−1.732170
233.N	0.548429	−5.909640	−1.557838
234.C	1.795771	−5.407817	−1.534556
235.H	6.273795	−7.824833	1.186532
236.H	6.805538	−9.343065	0.394344
237.H	4.467707	−9.513341	0.876016
238.H	5.325122	−9.926111	−1.777563
239.O	4.781492	−7.686043	−2.935859
240.H	3.079273	−8.796459	−2.865607
241.H	2.082228	−7.894745	−0.918754
242.H	5.051007	−5.445603	−1.235492
243.H	−0.885771	−2.916148	−1.728249
244.H	−2.476013	−4.642642	−1.656628
245.H	−1.927676	−6.303793	−1.599867
246.O	−3.539935	10.651471	−1.147996
247.C	−3.809850	8.395594	−2.161374
248.C	−3.102220	7.526038	−1.082798
249.C	0.404532	4.968684	−1.652336
250.H	−6.805538	9.343065	0.394344
251.H	−4.467707	9.513341	0.876016
252.H	−2.763933	10.384218	−0.620774
253.C	−6.439278	1.552577	1.524094
254.H	8.497858	9.954930	−0.745564
255.N	−2.983966	6.115167	−1.379180
256.H	−7.823270	−6.302414	1.195121
257.H	−5.325122	9.926111	−1.777563
258.H	−2.034327	−9.967662	1.890729
259.H	2.034327	9.967662	1.890729
260.H	−9.944579	8.494899	−0.698296
261.N	6.195533	−2.926863	1.560576
262.C	−1.551990	−6.438566	1.472333
263.H	9.973673	−2.054548	1.961268
264.H	9.944579	−8.494899	−0.698296
265.H	5.579348	−7.553018	−2.381542
266.H	7.577390	5.563840	−2.366790
267.H	−5.579348	7.553018	−2.381542
268.H	−7.577390	−5.563840	−2.366790
269.H	−7.626843	4.773166	−1.691333
270.H	−4.786121	−7.620280	−1.725780

271.H	7.626843	−4.773166	−1.691333
272.H	4.786121	7.620280	−1.725780
273.K	0.000000	0.000000	−0.051564

$_{RNA}$GQ-Rb^{+} -39433.62 (Symmetry C2)

1.C	6.480302	−1.477401	1.471349
2.N	5.359596	−0.784749	1.530511
3.C	4.338319	−1.731608	1.597210
4.C	2.925505	−1.584480	1.619071
5.O	2.262244	−0.517055	1.605653
6.N	2.259451	−2.827891	1.635982
7.C	2.887504	−4.062141	1.667365
8.N	2.122149	−5.169754	1.720605
9.N	4.220085	−4.194461	1.656293
10.C	4.873348	−3.025569	1.600000
11.H	10.748902	−3.548752	3.143928
12.H	11.508403	−4.371067	1.760480
13.H	9.482692	−5.537937	2.462297
14.H	9.929957	−4.953155	−0.248239
15.H	8.462419	−3.012314	−0.096114
16.O	7.098642	−4.275843	−1.039886
17.H	6.586714	−4.859623	1.480761
18.H	7.477142	−1.064082	1.410139
19.H	1.221735	−2.777219	1.641578
20.H	1.093529	−5.158100	1.613172
21.H	2.613505	−6.047328	1.574334
22.P	8.130909	−7.208708	−0.851499
23.O	8.825418	−8.633753	−0.653476
24.O	8.343444	−6.510608	−2.153722
25.O	6.584356	−7.584831	−0.658256
26.C	6.080150	−8.261772	0.561364
27.C	−3.096128	−1.178432	−1.933009
28.C	4.648858	−8.720557	0.338443
29.O	3.747310	−7.573266	0.300201
30.C	4.382652	−9.527538	−0.957671
31.O	3.508924	−10.651226	−0.729486
32.C	3.764177	−8.489000	−1.931657
33.C	3.024013	−7.528384	−0.955269
34.C	−4.338319	1.731608	1.597210
35.N	2.937674	−6.143296	−1.365587
36.C	−2.925505	1.584480	1.619071
37.H	−4.620672	2.502859	−1.748007
38.N	−3.624837	0.126795	−1.882800
39.N	−5.170320	−2.122919	1.724963
40.H	−6.277443	1.972743	−1.581400
41.C	−4.969584	0.432566	−1.736922
42.O	−7.843214	−4.716699	−2.784025
43.O	−1.859348	−1.355426	−2.078136
44.H	−8.953223	−3.023712	−2.608274
45.C	7.960724	−3.979772	0.049235
46.N	−2.854335	−6.249006	1.485925
47.H	−5.479876	−5.012461	−1.233311
48.H	−9.146251	−6.737495	0.710675
49.H	−9.957066	−5.278148	−1.416105
50.O	−7.098642	4.275843	−1.039886
51.C	3.983817	−5.220190	−1.417499
52.N	3.554273	−3.999592	−1.664145
53.O	−0.517758	−2.261880	1.606507
54.C	−4.062748	−2.887971	1.663669
55.C	−3.784375	−10.640888	2.042975
56.N	−2.828639	−2.259492	1.636972
57.C	7.182388	−3.945052	1.374270
58.C	−5.425779	−1.761804	−1.578588
59.O	−2.262244	0.517055	1.605653
60.H	−10.052942	1.934748	1.714938
61.N	−5.359596	0.784749	1.530511
62.N	−4.194895	−4.220360	1.642102
63.C	−3.025860	−4.873083	1.581330
64.N	−5.314457	1.732003	−1.781147
65.O	2.567292	10.652978	1.262250
66.C	3.784375	10.640888	2.042975
67.C	4.621233	9.382691	1.838785
68.O	3.871010	8.214036	2.339793
69.C	4.983172	9.061452	0.372732
70.O	6.370379	8.549679	0.402633
71.C	3.977091	7.957707	0.014110
72.C	3.945821	7.180140	1.339352
73.N	2.854335	6.249006	1.485925
74.C	1.477717	6.478888	1.440662
75.N	0.785148	5.358746	1.509852
76.C	1.732031	4.338051	1.584219
77.C	1.584969	2.925405	1.615754
78.O	0.517758	2.261880	1.606507
79.N	2.828639	2.259492	1.636972
80.C	4.062748	2.887971	1.663669
81.N	5.170320	2.122919	1.724963
82.N	4.194895	4.220360	1.642102
83.C	3.025860	4.873083	1.581330
84.H	3.559062	10.747869	3.110859
85.H	4.372272	11.505985	1.721274
86.H	5.544260	9.480340	2.421008
87.H	4.946687	9.927605	−0.287124
88.H	3.009048	8.458714	−0.130056
89.O	4.272855	7.094367	−1.073795
90.H	4.860035	6.583361	1.442941
91.H	1.063921	7.474993	1.370840
92.H	2.777862	1.221772	1.647227
93.H	5.159269	1.093485	1.624397
94.H	6.048293	2.613180	1.578167
95.P	7.203854	8.138634	−0.901910
96.O	8.623184	8.848391	−0.712660
97.O	6.498760	8.344738	−2.201249
98.O	7.596671	6.596256	−0.707606
99.C	8.277836	6.104537	0.514825
100.C	8.722871	4.666345	0.311465
101.O	7.566556	3.775869	0.286172
102.C	9.527198	4.374064	−0.980773
103.O	10.643633	3.494061	−0.739906
104.C	8.482305	3.750707	−1.944687
105.C	7.520308	3.030066	−0.955608
106.N	6.135310	2.939471	−1.364576
107.C	5.212786	3.985184	−1.427833
108.N	3.993104	3.553764	−1.676006
109.C	4.098351	2.167149	−1.770653
110.C	3.096128	1.178432	−1.933009

111.O	1.859348	1.355426	-2.078136
112.N	3.624837	-0.126795	-1.882800
113.C	4.969584	-0.432566	-1.736922
114.N	5.314457	-1.732003	-1.781147
115.N	5.912820	0.508511	-1.575841
116.C	5.425779	1.761804	-1.578588
117.H	7.566419	6.169519	1.341137
118.H	9.146251	6.737495	0.710675
119.H	9.332695	4.411302	1.186403
120.H	9.957066	5.278148	-1.416105
121.O	7.843214	4.716699	-2.784025
122.H	8.953223	3.023712	-2.608274
123.H	7.859541	2.001168	-0.789094
124.H	5.479876	5.012461	-1.233311
125.H	2.927705	-0.889675	-1.979170
126.H	4.620672	-2.502859	-1.748007
127.H	6.277443	-1.972743	-1.581400
128.O	-4.734822	7.846625	-2.763066
129.H	-3.048529	8.967353	-2.602038
130.O	-2.567292	-10.652978	1.262250
131.H	-1.992854	7.869428	-0.806571
132.H	-5.009469	5.487735	-1.215458
133.H	0.886409	2.931258	-1.987658
134.H	2.500841	4.623420	-1.766320
135.H	1.973284	6.281654	-1.608326
136.H	-6.586714	4.859623	1.480761
137.H	-7.477142	1.064082	1.410139
138.H	2.716464	-10.353431	-0.244772
139.H	-1.221735	2.777219	1.641578
140.C	-3.983817	5.220190	-1.417499
141.N	-3.554273	3.999592	-1.664145
142.C	-2.168356	4.104417	-1.768466
143.C	-1.181002	3.101109	-1.931013
144.O	-1.359491	1.863712	-2.069193
145.N	1.731062	5.318282	-1.804516
146.N	-0.508149	5.919024	-1.591005
147.C	-1.761589	5.432516	-1.584452
148.H	-6.126300	7.543160	1.382619
149.H	-1.093529	5.158100	1.613172
150.H	10.341121	2.714399	-0.237579
151.H	-2.613505	6.047328	1.574334
152.P	-8.130909	7.208708	-0.851499
153.O	-8.825418	8.633753	-0.653476
154.O	-8.343444	6.510608	-2.153722
155.O	-6.584356	7.584831	-0.658256
156.C	-6.080150	8.261772	0.561364
157.N	0.124539	3.629150	-1.890110
158.H	-8.575635	-9.820668	-0.618222
159.C	-4.648858	8.720557	0.338443
160.O	-3.747310	7.573266	0.300201
161.C	-4.382652	9.527538	-0.957671
162.C	-3.945821	-7.180140	1.339352
163.N	-0.785148	-5.358746	1.509852
164.C	-1.732031	-4.338051	1.584219
165.H	-7.859541	-2.001168	-0.789094
166.C	-1.584969	-2.925405	1.615754
167.H	-3.559062	-10.747869	3.110859
168.H	-4.372272	-11.505985	1.721274
169.H	-5.544260	-9.480340	2.421008
170.H	-3.009048	-8.458714	-0.130056
171.O	-4.272855	-7.094367	-1.073795
172.H	-4.860035	-6.583361	1.442941
173.H	-1.063921	-7.474993	1.370840
174.O	-10.658836	2.567546	1.289422
175.H	-9.332695	-4.411302	1.186403
176.H	-2.927705	0.889675	-1.979170
177.H	-2.777862	-1.221772	1.647227
178.H	-5.159269	-1.093485	1.624397
179.H	-6.048293	-2.613180	1.578167
180.P	-7.203854	-8.138634	-0.901910
181.O	-8.623184	-8.848391	-0.712660
182.O	-6.498760	-8.344738	-2.201249
183.N	-2.259451	2.827891	1.635982
184.O	-7.596671	-6.596256	-0.707606
185.C	-8.277836	-6.104537	0.514825
186.C	-8.722871	-4.666345	0.311465
187.O	-7.566556	-3.775869	0.286172
188.C	-9.527198	-4.374064	-0.980773
189.O	-10.643633	-3.494061	-0.739906
190.C	-8.482305	-3.750707	-1.944687
191.O	-6.370379	-8.549679	0.402633
192.C	-10.643590	3.780198	2.077203
193.N	-5.912820	-0.508511	-1.575841
194.C	-9.385097	4.617290	1.876182
195.O	-8.216126	3.865278	2.374278
196.C	-3.977091	-7.957707	0.014110
197.C	-7.520308	-3.030066	-0.955608
198.N	-6.135310	-2.939471	-1.364576
199.C	-5.212786	-3.985184	-1.427833
200.C	-9.063501	4.985571	0.411684
201.H	-4.946687	-9.927605	-0.287124
202.O	-8.550555	6.372432	0.448405
203.C	-7.960724	3.979772	0.049235
204.C	-7.182388	3.945052	1.374270
205.N	-3.993104	-3.553764	-1.676006
206.C	-2.887504	4.062141	1.667365
207.N	-2.122149	5.169754	1.720605
208.N	-4.220085	4.194461	1.656293
209.C	-4.873348	3.025569	1.600000
210.H	-10.748902	3.548752	3.143928
211.C	-4.098351	-2.167149	-1.770653
212.C	-4.621233	-9.382691	1.838785
213.O	-3.871010	-8.214036	2.339793
214.N	-6.250078	2.853909	1.516101
215.C	-4.983172	-9.061452	0.372732
216.H	-11.508403	4.371067	1.760480
217.O	10.658836	-2.567546	1.289422
218.H	-9.482692	5.537937	2.462297
219.C	10.643590	-3.780198	2.077203
220.C	9.385097	-4.617290	1.876182
221.O	8.216126	-3.865278	2.374278
222.H	-9.929957	4.953155	-0.248239
223.C	9.063501	-4.985571	0.411684
224.H	-8.462419	3.012314	-0.096114
225.H	-10.341121	-2.714399	-0.237579
226.O	8.550555	-6.372432	0.448405
227.C	2.168356	-4.104417	-1.768466
228.C	1.181002	-3.101109	-1.931013
229.O	1.359491	-1.863712	-2.069193

230.N	−0.124539	−3.629150	−1.890110
231.C	−0.431582	−4.974621	−1.752284
232.N	−1.731062	−5.318282	−1.804516
233.N	0.508149	−5.919024	−1.591005
234.C	1.761589	−5.432516	−1.584452
235.H	6.126300	−7.543160	1.382619
236.H	6.717294	−9.123287	0.773874
237.H	4.386474	−9.332441	1.209421
238.H	5.296737	−9.949575	−1.379545
239.O	4.734822	−7.846625	−2.763066
240.H	3.048529	−8.967353	−2.602038
241.H	1.992854	−7.869428	−0.806571
242.H	5.009469	−5.487735	−1.215458
243.H	−0.886409	−2.931258	−1.987658
244.H	−2.500841	−4.623420	−1.766320
245.H	−1.973284	−6.281654	−1.608326
246.O	−3.508924	10.651226	−0.729486
247.C	−3.764177	8.489000	−1.931657
248.C	−3.024013	7.528384	−0.955269
249.C	0.431582	4.974621	−1.752284
250.H	−6.717294	9.123287	0.773874
251.H	−4.386474	9.332441	1.209421
252.H	−2.716464	10.353431	−0.244772
253.C	−6.480302	1.477401	1.471349
254.H	8.575635	9.820668	−0.618222
255.N	−2.937674	6.143296	−1.365587
256.H	−7.566419	−6.169519	1.341137
257.H	−5.296737	9.949575	−1.379545
258.H	−1.939647	−10.043436	1.690248
259.H	1.939647	10.043436	1.690248
260.H	−9.799420	8.598003	−0.572653
261.N	6.250078	−2.853909	1.516101
262.C	−1.477717	−6.478888	1.440662
263.H	10.052942	−1.934748	1.714938
264.H	9.799420	−8.598003	−0.572653
265.H	5.521600	−7.643846	−2.214606
266.H	7.645026	5.510149	−2.243335
267.H	−5.521600	7.643846	−2.214606
268.H	−7.645026	−5.510149	−2.243335
269.H	−7.587296	4.820529	−1.698964
270.H	−4.807086	−7.586888	−1.738289
271.H	7.587296	−4.820529	−1.698964
272.H	4.807086	7.586888	−1.738289
273.Rb	0.000000	0.000000	−0.212342

RNAGQ-Cs^+ (Bond Energy: -39427.21) (Symmetry C2)

1.C	6.496925	−1.463861	1.476526
2.N	5.379101	−0.772673	1.586839
3.C	4.360678	−1.721767	1.666674
4.C	2.950668	−1.575484	1.754943
5.O	2.287216	−0.508903	1.803792
6.N	2.283477	−2.819542	1.756769
7.C	2.911242	−4.054739	1.731498
8.N	2.147227	−5.163624	1.782198
9.N	4.242659	−4.185851	1.670739
10.C	4.894574	−3.015549	1.622160
11.H	10.796016	−3.520649	3.041759
12.H	11.531785	−4.336172	1.641647
13.H	9.529372	−5.515425	2.387201
14.H	9.918319	−4.939571	−0.331750
15.H	8.455129	−2.996765	−0.152634
16.O	7.075150	−4.259147	−1.073718
17.H	6.605373	−4.845829	1.452319
18.H	7.491270	−1.048953	1.390962
19.H	1.247195	−2.771565	1.804577
20.H	1.117225	−5.153032	1.693649
21.H	2.636754	−6.037402	1.607486
22.P	8.101731	−7.197704	−0.889338
23.O	8.797093	−8.623634	−0.702260
24.O	8.285330	−6.506033	−2.199319
25.O	6.559518	−7.570269	−0.656120
26.C	6.084838	−8.227015	0.585951
27.C	−3.124070	−1.192618	−2.097450
28.C	4.646864	−8.684459	0.408526
29.O	3.748450	−7.534426	0.367369
30.C	4.344953	−9.517886	−0.862403
31.O	3.470140	−10.630487	−0.588825
32.C	3.710607	−8.496803	−1.844754
33.C	2.999894	−7.508390	−0.872187
34.C	−4.360678	1.721767	1.666674
35.N	2.919925	−6.132054	−1.312861
36.C	−2.950668	1.575484	1.754943
37.H	−4.607270	2.507698	−1.810716
38.N	−3.638646	0.118874	−2.025882
39.N	−5.163897	−2.145411	1.779917
40.H	−6.254489	1.987425	−1.564082
41.C	−4.969287	0.437376	−1.789880
42.O	−7.881959	−4.668522	−2.716035
43.O	−1.904493	−1.382961	−2.340540
44.H	−8.984526	−2.976938	−2.494316
45.C	7.955618	−3.964072	0.000868
46.N	−2.841230	−6.266138	1.499581
47.H	−5.487161	−4.996658	−1.189544
48.H	−9.101201	−6.723285	0.787512
49.H	−9.960658	−5.245144	−1.303245
50.O	−7.075150	4.259147	−1.073718
51.C	3.972668	−5.220501	−1.407293
52.N	3.553399	−4.012654	−1.724885
53.O	−0.509279	−2.285281	1.802654
54.C	−4.055180	−2.909487	1.727909
55.C	−3.770079	−10.668087	1.997292
56.N	−2.819902	−2.281695	1.753976
57.C	7.199163	−3.931044	1.337990
58.C	−5.429725	−1.751653	−1.579231
59.O	−2.287216	0.508903	1.803792
60.H	−10.063792	1.907341	1.632800
61.N	−5.379101	0.772673	1.586839
62.N	−4.185914	−4.240937	1.666929
63.C	−3.015425	−4.892750	1.620277
64.N	−5.304825	1.739391	−1.812813
65.O	2.560830	10.676124	1.204404
66.C	3.770079	10.668087	1.997292
67.C	4.605364	9.405315	1.816215
68.O	3.851104	8.244048	2.328826
69.C	4.976257	9.062924	0.357109

70.O	6.361574	8.546791	0.404953
71.C	3.967851	7.958065	0.007589
72.C	3.931172	7.197439	1.342211
73.N	2.841230	6.266138	1.499581
74.C	1.463807	6.495476	1.479443
75.N	0.772554	5.377548	1.588506
76.C	1.721653	4.358911	1.665719
77.C	1.575631	2.948794	1.752959
78.O	0.509279	2.285281	1.802654
79.N	2.819902	2.281695	1.753976
80.C	4.055180	2.909487	1.727909
81.N	5.163897	2.145411	1.779917
82.N	4.185914	4.240937	1.666929
83.C	3.015425	4.892750	1.620277
84.H	3.534508	10.788056	3.061441
85.H	4.364660	11.527238	1.671687
86.H	5.524695	9.509743	2.403074
87.H	4.948311	9.920169	-0.314602
88.H	3.002095	8.460644	-0.146005
89.O	4.262953	7.079879	-1.068695
90.H	4.845973	6.603439	1.456136
91.H	1.049307	7.490233	1.396966
92.H	2.772020	1.245221	1.802565
93.H	5.153719	1.115306	1.691649
94.H	6.038238	2.634665	1.607514
95.P	7.201906	8.105373	-0.884986
96.O	8.626302	8.804996	-0.697613
97.O	6.508561	8.293932	-2.193317
98.O	7.579106	6.563316	-0.658707
99.C	8.237861	6.086451	0.581714
100.C	8.690577	4.647343	0.402447
101.O	7.537609	3.752747	0.361709
102.C	9.522419	4.344358	-0.869442
103.O	10.634239	3.468036	-0.597456
104.C	8.499002	3.711902	-1.850371
105.C	7.511212	3.002364	-0.876613
106.N	6.134797	2.921605	-1.316818
107.C	5.223294	3.974283	-1.412135
108.N	4.015225	3.554675	-1.728422
109.C	4.117095	2.169014	-1.836469
110.C	3.124070	1.192618	-2.097450
111.O	1.904493	1.382961	-2.340540
112.N	3.638646	-0.118874	-2.025882
113.C	4.969287	-0.437376	-1.789880
114.N	5.304825	-1.739391	-1.812813
115.N	5.907244	0.494937	-1.564533
116.C	5.429725	1.751653	-1.579231
117.H	7.510630	6.158517	1.393440
118.H	9.101201	6.723285	0.787512
119.H	9.281430	4.402260	1.292955
120.H	9.960658	5.245144	-1.303245
121.O	7.881959	4.668522	-2.716035
122.H	8.984526	2.976938	-2.494316
123.H	7.838184	1.971306	-0.698790
124.H	5.487161	4.996658	-1.189544
125.H	2.951378	-0.877312	-2.189400
126.H	4.607270	-2.507698	-1.810716
127.H	6.254489	-1.987425	-1.564082
128.O	-4.665676	7.879506	-2.711706
129.H	-2.976391	8.984789	-2.487826
130.O	-2.560830	-10.676124	1.204404
131.H	-1.968620	7.835065	-0.695355
132.H	-4.994715	5.484019	-1.183047
133.H	0.878485	2.949260	-2.190280
134.H	2.508696	4.606662	-1.813548
135.H	1.987356	6.252642	-1.563918
136.H	-6.605373	4.845829	1.452319
137.H	-7.491270	1.048953	1.390962
138.H	2.686630	-10.315988	-0.100042
139.H	-1.247195	2.771565	1.804577
140.C	-3.972668	5.220501	-1.407293
141.N	-3.553399	4.012654	-1.724885
142.C	-2.167875	4.114707	-1.834650
143.C	-1.191719	3.122227	-2.097861
144.O	-1.382512	1.902773	-2.342019
145.N	1.740173	5.303833	-1.816909
146.N	-0.493749	5.904859	-1.564551
147.C	-1.750328	5.427157	-1.577083
148.H	-6.154596	7.496591	1.394995
149.H	-1.117225	5.153032	1.693649
150.H	10.319646	2.685840	-0.106597
151.H	-2.636754	6.037402	1.607486
152.P	-8.101731	7.197704	-0.889338
153.O	-8.797093	8.623634	-0.702260
154.O	-8.285330	6.506033	-2.199319
155.O	-6.559518	7.570269	-0.656120
156.C	-6.084838	8.227015	0.585951
157.N	0.119836	3.636407	-2.026647
158.H	-8.589387	-9.781008	-0.645013
159.C	-4.646864	8.684459	0.408526
160.O	-3.748450	7.534426	0.367369
161.C	-4.344953	9.517886	-0.862403
162.C	-3.931172	-7.197439	1.342211
163.N	-0.772554	-5.377548	1.588506
164.C	-1.721653	-4.358911	1.665719
165.H	-7.838184	-1.971306	-0.698790
166.C	-1.575631	-2.948794	1.752959
167.H	-3.534508	-10.788056	3.061441
168.H	-4.364660	-11.527238	1.671687
169.H	-5.524695	-9.509743	2.403074
170.H	-3.002095	-8.460644	-0.146005
171.O	-4.262953	-7.079879	-1.068695
172.H	-4.845973	-6.603439	1.456136
173.H	-1.049307	-7.490233	1.396966
174.O	-10.661549	2.537050	1.191554
175.H	-9.281430	-4.402260	1.292955
176.H	-2.951378	0.877312	-2.189400
177.H	-2.772020	-1.245221	1.802565
178.H	-5.153719	-1.115306	1.691649
179.H	-6.038238	-2.634665	1.607514
180.P	-7.201906	-8.105373	-0.884986
181.O	-8.626302	-8.804996	-0.697613
182.O	-6.508561	-8.293932	-2.193317
183.N	-2.283477	2.819542	1.756769
184.O	-7.579106	-6.563316	-0.658707
185.C	-8.237861	-6.086451	0.581714
186.C	-8.690577	-4.647343	0.402447
187.O	-7.537609	-3.752747	0.361709
188.C	-9.522419	-4.344358	-0.869442

189.O	−10.634239	−3.468036	−0.597456
190.C	−8.499002	−3.711902	−1.850371
191.O	−6.361574	−8.546791	0.404953
192.C	−10.670072	3.751083	1.977076
193.N	−5.907244	−0.494937	−1.564533
194.C	−9.413268	4.596730	1.801549
195.O	−8.248461	3.852862	2.322106
196.C	−3.967851	−7.958065	0.007589
197.C	−7.511212	−3.002364	−0.876613
198.N	−6.134797	−2.921605	−1.316818
199.C	−5.223294	−3.974283	−1.412135
200.C	−9.064650	4.969294	0.344689
201.H	−4.948311	−9.920169	−0.314602
202.O	−8.551769	6.355996	0.396777
203.C	−7.955618	3.964072	0.000868
204.C	−7.199163	3.931044	1.337990
205.N	−4.015225	−3.554675	−1.728422
206.C	−2.911242	4.054739	1.731498
207.N	−2.147227	5.163624	1.782198
208.N	−4.242659	4.185851	1.670739
209.C	−4.894574	3.015549	1.622160
210.H	−10.796016	3.520649	3.041759
211.C	−4.117095	−2.169014	−1.836469
212.C	−4.605364	−9.405315	1.816215
213.O	−3.851104	−8.244048	2.328826
214.N	−6.267939	2.841331	1.499588
215.C	−4.976257	−9.062924	0.357109
216.H	−11.531785	4.336172	1.641647
217.O	10.661549	−2.537050	1.191554
218.H	−9.529372	5.515425	2.387201
219.C	10.670072	−3.751083	1.977076
220.C	9.413268	−4.596730	1.801549
221.O	8.248461	−3.852862	2.322106
222.H	−9.918319	4.939571	−0.331750
223.C	9.064650	−4.969294	0.344689
224.H	−8.455129	2.996765	−0.152634
225.H	−10.319646	−2.685840	−0.106597
226.O	8.551769	−6.355996	0.396777
227.C	2.167875	−4.114707	−1.834650
228.C	1.191719	−3.122227	−2.097861
229.O	1.382512	−1.902773	−2.342019
230.N	−0.119836	−3.636407	−2.026647
231.C	−0.438238	−4.967214	−1.791915
232.N	−1.740173	−5.303833	−1.816909
233.N	0.493749	−5.904859	−1.564551
234.C	1.750328	−5.427157	−1.577083
235.H	6.154596	−7.496591	1.394995
236.H	6.724215	−9.087680	0.794993
237.H	4.404278	−9.275308	1.299668
238.H	5.246320	−9.954949	−1.295894
239.O	4.665676	−7.879506	−2.711706
240.H	2.976391	−8.984789	−2.487826
241.H	1.968620	−7.835065	−0.695355
242.H	4.994715	−5.484019	−1.183047
243.H	−0.878485	−2.949260	−2.190280
244.H	−2.508696	−4.606662	−1.813548
245.H	−1.987356	−6.252642	−1.563918
246.O	−3.470140	10.630487	−0.588825
247.C	−3.710607	8.496803	−1.844754
248.C	−2.999894	7.508390	−0.872187
249.C	0.438238	4.967214	−1.791915
250.H	−6.724215	9.087680	0.794993
251.H	−4.404278	9.275308	1.299668
252.H	−2.686630	10.315988	−0.100042
253.C	−6.496925	1.463861	1.476526
254.H	8.589387	9.781008	−0.645013
255.N	−2.919925	6.132054	−1.312861
256.H	−7.510630	−6.158517	1.393440
257.H	−5.246320	9.954949	−1.295894
258.H	−1.923457	−10.079519	1.636128
259.H	1.923457	10.079519	1.636128
260.H	−9.774019	8.592272	−0.666558
261.N	6.267939	−2.841331	1.499588
262.C	−1.463807	−6.495476	1.479443
263.H	10.063792	−1.907341	1.632800
264.H	9.774019	−8.592272	−0.666558
265.H	5.464596	−7.666015	−2.185129
266.H	7.671642	5.468175	−2.189313
267.H	−5.464596	7.666015	−2.185129
268.H	−7.671642	−5.468175	−2.189313
269.H	−7.549109	4.812316	−1.736557
270.H	−4.811860	−7.556823	−1.732831
271.H	7.549109	−4.812316	−1.736557
272.H	4.811860	7.556823	−1.732831
273.Cs	0.000000	0.000000	−0.277420

Table S4. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of guanosine dimer (guanosine monophosphate + guanosine), guanosine dimer counterion (Na^+), and $(H_2CO)_8$ at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

Guanosine dimer (Bond Energy: -9837.28) (Symmetry C1) (imag freq -14cm-1)			
1.C	−8.916515	−4.838006	0.112362
2.O	−2.875119	−7.929217	2.536158
3.O	−9.816387	−3.793548	0.542949
4.C	−7.946894	−4.334398	−0.985480
5.O	−5.567617	−8.911222	1.342342
6.H	−6.914663	−6.732824	2.310814
7.N	−5.297388	−1.066928	−0.476094
8.C	−4.165877	−9.268526	1.019046
9.H	−5.681879	−2.925349	2.521218
10.C	−3.446930	−8.141477	0.261693
11.H	−0.701450	−10.871150	1.502129
12.C	−6.859653	−3.641241	−0.122438
13.N	−5.553732	−3.488924	−0.724383
14.C	−4.704397	−4.488070	−1.208985
15.C	−1.016008	−6.114579	0.651431
16.O	−1.402561	−10.207283	1.374878
17.H	−4.163664	−10.225851	0.498921
18.C	−3.650309	−2.624601	−1.472286
19.H	−7.793446	−10.480585	1.167756
20.O	−7.247175	−7.266754	0.308976
21.C	−7.705528	−6.625730	1.565089

22.N	−3.567270	−4.003503	−1.668047
23.C	−3.269703	−7.123744	1.400712
24.N	−0.450289	−4.921893	0.601214
25.C	−1.403806	−4.040475	1.120328
26.H	−7.198460	−2.633002	0.141394
27.C	−2.711262	−1.588032	−1.759710
28.C	−1.389503	−2.620364	1.289964
29.H	−1.794292	−10.161546	3.440569
30.H	−2.784838	−11.318189	2.509840
31.H	−4.144585	−9.468907	3.171539
32.H	−2.466640	−8.543511	−0.024021
33.O	−4.107367	−7.568043	−0.859328
34.P	−6.744744	−8.786579	0.262257
35.H	−4.219510	−6.613005	1.597839
36.C	−7.988565	−5.157339	1.309135
37.H	−4.002789	1.896796	−0.376113
38.N	−3.198706	−0.326665	−1.319644
39.N	−4.851042	−2.340426	2.599417
40.H	−5.541641	1.341935	0.177339
41.C	−4.419623	−0.094635	−0.720652
42.O	−7.456610	−5.395029	−1.813349
43.O	−1.594876	−1.665201	−2.306042
44.H	−8.427492	−3.612311	−1.648611
45.H	−0.563180	−7.043805	0.333527
46.N	−2.306740	−6.070079	1.181293
47.H	−4.950503	−5.535750	−1.145514
48.H	−8.612878	−7.133766	1.898770
49.H	−9.475147	−5.713983	−0.231849
50.C	−3.424232	−9.287000	2.367131
51.O	−6.732866	−4.456718	1.068047
52.H	−8.446526	−4.762499	2.224782
53.O	−0.481130	−1.803778	1.047234
54.C	−3.724719	−2.945173	2.119613
55.C	−2.318575	−10.323335	2.489688
56.N	−2.638463	−2.155503	1.800979
57.H	−2.582811	0.463133	−1.502838
58.C	−4.871561	−2.287657	−0.872186
59.H	−10.448617	−3.632895	−0.182278
60.O	−7.978167	−9.548571	0.934985
61.O	−6.364294	−9.176867	−1.128360
62.N	−3.705319	−4.264762	1.997332
63.C	−2.555875	−4.742017	1.489214
64.N	−4.726252	1.188732	−0.404105
65.H	−2.692713	−1.151531	1.960497
66.H	−5.000257	−1.363239	2.370199
67.H	−7.281714	−6.174248	−1.243344
68.H	−4.739668	−8.224349	−1.233415

Counterion Guanosine dimer (Bond Energy: -9834.18) (Symmetry C1)			
1.C	−8.922753	−5.425376	0.160584
2.O	−2.929522	−6.687472	3.003056
3.O	−9.829814	−4.310604	0.312682
4.C	−7.981277	−5.239977	−1.052740
5.O	−5.318389	−8.519769	2.435453
6.H	−6.932808	−6.637742	2.802509
7.N	−5.578187	−1.766500	−1.348059
8.C	−3.890648	−8.733590	2.202926
9.H	−5.484746	−1.885886	2.136557
10.C	−3.342015	−7.911734	1.021757
11.H	−0.167867	−9.326224	3.088289
12.C	−6.906709	−4.317423	−0.426903
13.N	−5.652660	−4.204123	−1.135869
14.C	−4.779844	−5.218071	−1.540820
15.C	−1.252333	−5.765824	0.334375
16.O	−0.977975	−8.910267	2.743243
17.H	−3.691995	−9.802729	2.105866
18.C	−3.913841	−3.368212	−2.236968
19.H	−4.706363	−8.706644	−0.181165
20.O	−7.249624	−7.706292	1.027836
21.C	−7.705999	−6.744429	2.036879
22.N	−3.738697	−4.751523	−2.203746
23.C	−3.351637	−6.494518	1.628787
24.N	−0.688410	−4.650103	−0.089490
25.C	−1.556585	−3.631517	0.305862
26.H	−7.307873	−3.299373	−0.351525
27.C	−3.104847	−2.343314	−2.814472
28.C	−1.477153	−2.215768	0.129454
29.H	−1.435743	−8.133432	4.641434
30.H	−2.147645	−9.730512	4.288428
31.H	−3.861226	−8.072492	4.258433
32.H	−2.300610	−8.234983	0.907229
33.O	−4.010355	−7.995357	−0.229177
34.P	−6.525117	−9.091746	1.504813
35.H	−4.356607	−6.058528	1.593659
36.C	−7.954872	−5.404519	1.372316
37.H	−4.700488	1.226058	−2.173076
38.N	−3.644856	−1.056878	−2.537476
39.N	−4.631969	−1.402202	1.874963
40.H	−6.061621	0.685199	−1.277198
41.C	−4.806148	−0.801214	−1.838981
42.O	−7.463998	−6.492335	−1.519473
43.O	−2.055439	−2.446803	−3.476951
44.H	−8.480324	−4.758220	−1.896030
45.H	−0.851005	−6.760557	0.203523
46.N	−2.464272	−5.541078	0.988653
47.H	−4.937556	−6.249859	−1.269818
48.H	−8.629756	−7.113529	2.493617
49.H	−9.477302	−6.366028	0.084006
50.C	−3.178471	−8.084695	3.402494
51.O	−6.681532	−4.872034	0.889430
52.H	−8.362148	−4.727635	2.134477
53.O	−0.589769	−1.535291	−0.417618
54.C	−3.655016	−2.195238	1.349300
55.C	−1.890018	−8.753021	3.856910
56.N	−2.621830	−1.572109	0.679678
57.H	−3.105572	−0.273617	−2.901155
58.C	−5.089935	−3.008677	−1.564872
59.H	−10.487465	−4.366497	−0.405512
60.O	−7.456205	−9.932301	2.352424
61.O	−5.990986	−9.759690	0.242312
62.N	−3.706939	−3.509674	1.524451
63.C	−2.659534	−4.166689	0.983714
64.N	−5.116839	0.502806	−1.597544
65.H	−2.616173	−0.555987	0.615101
66.H	−4.768391	−0.475296	1.486830

67.H	−7.250207	−7.044295	−0.732128
68.Na	−7.258151	−11.763893	0.784607

$(H_2CO)_8$ (Bond Energy: -3976.89) (Symmetry C2)			
1.O	2.351634	0.139469	−2.327449
2.O	0.140701	−2.345611	−2.301209
3.C	−1.586184	2.927653	1.614022
4.C	−2.923026	−1.584300	1.612431
5.O	−1.677766	−1.639309	1.683388
6.C	−0.690750	−3.243043	−2.044596
7.C	1.586184	−2.927653	1.614022
8.C	2.923026	1.584300	1.612431
9.C	−3.247179	0.691344	−2.060590
10.O	1.641432	−1.682350	1.688147
11.O	1.677766	1.639309	1.683388
12.O	−2.351634	−0.139469	−2.327449
13.C	0.690750	3.243043	−2.044596
14.C	3.247179	−0.691344	−2.060590
15.O	−1.641432	1.682350	1.688147
16.O	−0.140701	2.345611	−2.301209
17.H	−2.502335	3.546214	1.579509
18.H	−0.610461	3.446785	1.584426
19.H	−3.541758	−2.500520	1.579396
20.H	−3.443283	−0.609118	1.584085
21.H	−1.775654	−3.040904	−2.104776
22.H	−0.369084	−4.262320	−1.762705
23.H	0.610461	−3.446785	1.584426
24.H	2.502335	−3.546214	1.579509
25.H	3.443283	0.609118	1.584085
26.H	3.541758	2.500520	1.579396
27.H	−4.318410	0.431851	−2.150201
28.H	−2.985198	1.715877	−1.740484
29.H	0.369084	4.262320	−1.762705
30.H	1.775654	3.040904	−2.104776
31.H	2.985198	−1.715877	−1.740484
32.H	4.318410	−0.431851	−2.150201

Table S4. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of $_{RNA}GQ_{4Na}$-M^+ at the COSMO ZORA-BLYP-D3(BJ)/TZ2P level of theory.

$_{RNA}GQ_{4Na}$-Na^+ (Bond Energy: -39429.48) (Symmetry C2)			
1.C	1.788047	6.331377	1.948624
2.N	1.048514	5.252458	2.108210
3.C	1.943929	4.185411	2.170353
4.C	1.725679	2.779987	2.227198
5.O	0.629024	2.167665	2.248206
6.N	2.934404	2.058676	2.237470
7.C	4.195882	2.623652	2.196967
8.N	5.259697	1.799351	2.265104
9.N	4.396688	3.945516	2.111026
10.C	3.259044	4.655016	2.072998
11.H	4.990695	10.055431	3.946732
12.H	5.457710	10.994146	2.507951
13.H	6.435528	8.745937	2.454471
14.H	5.127856	9.809512	0.205298
15.H	3.121864	8.517742	0.725935
16.O	3.814682	7.306412	−0.805629
17.H	5.089237	6.233241	1.314641
18.H	1.416535	7.341667	1.851772
19.H	2.822593	1.023563	2.246583
20.H	5.187446	0.769369	2.160128
21.H	6.161828	2.228864	2.097922
22.P	6.932154	8.360240	−1.393948
23.O	7.865266	9.546738	−1.513417
24.O	5.748328	8.369406	−2.357634
25.O	7.700242	6.941718	−1.615186
26.C	8.808617	6.531178	−0.745966
27.C	1.267437	−3.014555	−0.926512
28.C	9.033980	5.037061	−0.905650
29.O	7.872730	4.318816	−0.377210
30.C	9.241279	4.536375	−2.361846
31.O	10.337701	3.605741	−2.476034
32.C	7.877713	3.899948	−2.730775
33.C	7.415997	3.355208	−1.349632
34.C	−1.943929	−4.185411	2.170353
35.N	5.987843	3.184376	−1.189572
36.C	−1.725679	−2.779987	2.227198
37.H	−2.326055	−4.699268	−1.053032
38.N	−0.004846	−3.610689	−0.926536
39.N	1.804726	−5.262827	2.228647
40.H	−1.743477	−6.345544	−1.187132
41.C	−0.249667	−4.966576	−1.091760
42.O	4.780960	−7.006350	−3.409820
43.O	1.381954	−1.769641	−0.782702
44.H	3.015792	−8.025795	−3.496926
45.C	4.002836	7.917196	0.461313
46.N	6.025464	−3.149695	1.775315
47.H	5.232459	−5.285286	−1.244011
48.H	7.070424	−9.748106	−1.193985
49.H	5.283093	−9.518071	−3.153276
50.O	−3.814682	−7.306412	−0.805629
51.C	5.021945	4.186578	−1.109389
52.N	3.805121	3.691532	−1.009981
53.O	2.167178	−0.632536	2.216829
54.C	2.625229	−4.198842	2.141583
55.C	10.111561	−4.928417	2.717867
56.N	2.060706	−2.937653	2.202696
57.C	4.258688	6.894830	1.585714
58.C	1.966501	−5.330543	−1.172134
59.O	−0.629024	−2.167665	2.248206
60.H	−2.934533	−9.765738	2.966829
61.N	−1.048514	−5.252458	2.108210
62.N	3.944491	−4.397796	2.016612
63.C	4.651262	−3.259100	1.967271
64.N	−1.529100	−5.355141	−1.170609
65.O	−10.425873	3.548981	2.416404

66.C	−10.111561	4.928417	2.717867
67.C	−8.837280	5.417513	2.039572
68.O	−7.693896	4.647774	2.566177
69.C	−8.791026	5.252326	0.503585
70.O	−8.095984	6.422948	−0.028971
71.C	−7.910659	4.001746	0.320883
72.C	−6.877035	4.260328	1.434934
73.N	−6.025464	3.149695	1.775315
74.C	−6.324985	1.787503	1.816323
75.N	−5.249944	1.048743	2.003920
76.C	−4.184135	1.944699	2.084504
77.C	−2.780528	1.728256	2.177563
78.O	−2.167178	0.632536	2.216829
79.N	−2.060706	2.937653	2.202696
80.C	−2.625229	4.198842	2.141583
81.N	−1.804726	5.262827	2.228647
82.N	−3.944491	4.397796	2.016612
83.C	−4.651262	3.259100	1.967271
84.H	−10.016164	5.073134	3.801575
85.H	−10.954766	5.525983	2.358269
86.H	−8.692788	6.476317	2.284457
87.H	−9.782942	5.160276	0.056266
88.H	−8.523448	3.134831	0.602639
89.O	−7.315585	3.782899	−0.948759
90.H	−6.207814	5.079000	1.147313
91.H	−7.333018	1.415657	1.700056
92.H	−1.026167	2.826544	2.240907
93.H	−0.770646	5.191221	2.178895
94.H	−2.228493	6.165620	2.051963
95.P	−8.324444	6.927218	−1.561283
96.O	−9.541807	7.819963	−1.678221
97.O	−8.295537	5.745167	−2.527105
98.O	−6.930329	7.738720	−1.779449
99.C	−6.537994	8.840781	−0.892905
100.C	−5.037810	9.054881	−1.005588
101.O	−4.344934	7.883753	−0.465043
102.C	−4.490985	9.270325	−2.444279
103.O	−3.553608	10.364113	−2.521871
104.C	−3.849220	7.906562	−2.802300
105.C	−3.349141	7.434275	−1.408338
106.N	−3.181185	6.005370	−1.253018
107.C	−4.183225	5.036138	−1.220923
108.N	−3.689347	3.819569	−1.115242
109.C	−2.305728	3.972433	−1.081652
110.C	−1.267437	3.014555	−0.926512
111.O	−1.381954	1.769641	−0.782702
112.N	0.004846	3.610689	−0.926536
113.C	0.249667	4.966576	−1.091760
114.N	1.529100	5.355141	−1.170609
115.N	−0.737268	5.873817	−1.189318
116.C	−1.966501	5.330543	−1.172134
117.H	−6.797595	8.580244	0.135939
118.H	−7.070424	9.748106	−1.193985
119.H	−4.788121	9.928179	−0.390219
120.H	−5.283093	9.518071	−3.153276
121.O	−4.780960	7.006350	−3.409820
122.H	−3.015792	8.025795	−3.496926
123.H	−2.372301	7.886661	−1.192625
124.H	−5.232459	5.285286	−1.244011
125.H	0.794108	2.941037	−0.840968
126.H	2.326055	4.699268	−1.053032
127.H	1.743477	6.345544	−1.187132
128.O	−6.969575	−4.844877	−3.304895
129.H	−7.996399	−3.087992	−3.450453
130.O	10.425873	−3.548981	2.416404
131.H	−7.869042	−2.371577	−1.168796
132.H	−5.272453	−5.235766	−1.094590
133.H	−2.921812	0.799451	−0.894496
134.H	−4.678617	2.324706	−1.164730
135.H	−6.320354	1.736771	−1.298862
136.H	−5.089237	−6.233241	1.314641
137.H	−1.416535	−7.341667	1.851772
138.H	10.233309	2.897369	−1.813592
139.H	−2.822593	−1.023563	2.246583
140.C	−5.021945	−4.186578	−1.109389
141.N	−3.805121	−3.691532	−1.009981
142.C	−3.954416	−2.307191	−1.031644
143.C	−2.996403	−1.265196	−0.903484
144.O	−1.753704	−1.377077	−0.736878
145.N	−5.329457	1.523837	−1.281415
146.N	−5.851406	−0.740660	−1.219333
147.C	−5.310809	−1.969160	−1.149464
148.H	−8.548815	−6.756467	0.291401
149.H	−5.187446	−0.769369	2.160128
150.H	−2.868785	10.256133	−1.835580
151.H	−6.161828	−2.228864	2.097922
152.P	−6.932154	−8.360240	−1.393948
153.O	−7.865266	−9.546738	−1.513417
154.O	−5.748328	−8.369406	−2.357634
155.O	−7.700242	−6.941718	−1.615186
156.C	−8.808617	−6.531178	−0.745966
157.N	−3.589944	0.006772	−0.962919
158.Na	−10.390111	6.456254	−3.486435
159.C	−9.033980	−5.037061	−0.905650
160.O	−7.872730	−4.318816	−0.377210
161.C	−9.241279	−4.536375	−2.361846
162.C	6.877035	−4.260328	1.434934
163.N	5.249944	−1.048743	2.003920
164.C	4.184135	−1.944699	2.084504
165.H	2.372301	−7.886661	−1.192625
166.C	2.780528	−1.728256	2.177563
167.H	10.016164	−5.073134	3.801575
168.H	10.954766	−5.525983	2.358269
169.H	8.692788	−6.476317	2.284457
170.H	8.523448	−3.134831	0.602639
171.O	7.315585	−3.782899	−0.948759
172.H	6.207814	−5.079000	1.147313
173.H	7.333018	−1.415657	1.700056
174.O	−3.485784	−10.443533	2.534379
175.H	4.788121	−9.928179	−0.390219
176.H	−0.794108	−2.941037	−0.840968
177.H	1.026167	−2.826544	2.240907
178.H	0.770646	−5.191221	2.178895
179.H	2.228493	−6.165620	2.051963
180.P	8.324444	−6.927218	−1.561283
181.O	9.541807	−7.819963	−1.678221
182.O	8.295537	−5.745167	−2.527105
183.N	−2.934404	−2.058676	2.237470
184.O	6.930329	−7.738720	−1.779449

185.C	6.537994	−8.840781	−0.892905
186.C	5.037810	−9.054881	−1.005588
187.O	4.344934	−7.883753	−0.465043
188.C	4.490985	−9.270325	−2.444279
189.O	3.553608	−10.364113	−2.521871
190.C	3.849220	−7.906562	−2.802300
191.O	8.095984	−6.422948	−0.028971
192.C	−4.863418	−10.145661	2.860384
193.N	0.737268	−5.873817	−1.189318
194.C	−5.378369	−8.875137	2.194599
195.O	−4.617177	−7.723544	2.716844
196.C	7.910659	−4.001746	0.320883
197.C	3.349141	−7.434275	−1.408338
198.N	3.181185	−6.005370	−1.253018
199.C	4.183225	−5.036138	−1.220923
200.C	−5.234506	−8.820937	0.656410
201.H	9.782942	−5.160276	0.056266
202.O	−6.426830	−8.150549	0.141029
203.C	−4.002836	−7.917196	0.461313
204.C	−4.258688	−6.894830	1.585714
205.N	3.689347	−3.819569	−1.115242
206.C	−4.195882	−2.623652	2.196967
207.N	−5.259697	−1.799351	2.265104
208.N	−4.396688	−3.945516	2.111026
209.C	−3.259044	−4.655016	2.072998
210.H	−4.990695	−10.055431	3.946732
211.C	2.305728	−3.972433	−1.081652
212.C	8.837280	−5.417513	2.039572
213.O	7.693896	−4.647774	2.566177
214.N	−3.150586	−6.033364	1.911476
215.C	8.791026	−5.252326	0.503585
216.H	−5.457710	−10.994146	2.507951
217.O	3.485784	10.443533	2.534379
218.H	−6.435528	−8.745937	2.454471
219.C	4.863418	10.145661	2.860384
220.C	5.378369	8.875137	2.194599
221.O	4.617177	7.723544	2.716844
222.H	−5.127856	−9.809512	0.205298
223.C	5.234506	8.820937	0.656410
224.H	−3.121864	−8.517742	0.725935
225.H	2.868785	−10.256133	−1.835580
226.O	6.426830	8.150549	0.141029
227.C	3.954416	2.307191	−1.031644
228.C	2.996403	1.265196	−0.903484
229.O	1.753704	1.377077	−0.736878
230.N	3.589944	−0.006772	−0.962919
231.C	4.943246	−0.247290	−1.149622
232.N	5.329457	−1.523837	−1.281415
233.N	5.851406	0.740660	−1.219333
234.C	5.310809	1.969160	−1.149464
235.H	8.548815	6.756467	0.291401
236.H	9.710893	7.080002	−1.032482
237.H	9.913644	4.775741	−0.304332
238.H	9.481113	5.351321	−3.047241
239.O	6.969575	4.844877	−3.304895
240.H	7.996399	3.087992	−3.450453
241.H	7.869042	2.371577	−1.168796
242.H	5.272453	5.235766	−1.094590
243.H	2.921812	−0.799451	−0.894496
244.H	4.678617	−2.324706	−1.164730
245.H	6.320354	−1.736771	−1.298862
246.O	−10.337701	−3.605741	−2.476034
247.C	−7.877713	−3.899948	−2.730775
248.C	−7.415997	−3.355208	−1.349632
249.C	−4.943246	0.247290	−1.149622
250.H	−9.710893	−7.080002	−1.032482
251.H	−9.913644	−4.775741	−0.304332
252.H	−10.233309	−2.897369	−1.813592
253.C	−1.788047	−6.331377	1.948624
254.H	−7.676118	4.441191	−1.606279
255.N	−5.987843	−3.184376	−1.189572
256.H	6.797595	−8.580244	0.135939
257.H	−9.481113	−5.351321	−3.047241
258.H	9.748600	−2.998085	2.850293
259.H	−9.748600	2.998085	2.850293
260.Na	−6.543673	−10.422865	−3.340250
261.N	3.150586	6.033364	1.911476
262.C	6.324985	−1.787503	1.816323
263.H	2.934533	9.765738	2.966829
264.Na	10.390111	−6.456254	−3.486435
265.H	7.059147	5.690949	−2.809298
266.H	−5.641080	7.096870	−2.939356
267.H	−7.059147	−5.690949	−2.809298
268.H	5.641080	−7.096870	−2.939356
269.H	−4.452661	−7.702310	−1.462923
270.H	7.676118	−4.441191	−1.606279
271.H	4.452661	7.702310	−1.462923
272.Na	6.543673	10.422865	−3.340250
273.Na	0.000000	0.000000	0.508428

$_{RNA}GQ_{4Na}$-K^+ (Bond Energy: -39432.58) (Symmetry C2)

1.C	1.802532	6.359649	1.889606
2.N	1.064482	5.292694	2.120980
3.C	1.958936	4.224410	2.184866
4.C	1.738847	2.828415	2.334268
5.O	0.641516	2.227204	2.453703
6.N	2.942367	2.096739	2.316255
7.C	4.204466	2.649713	2.186366
8.N	5.264405	1.820587	2.240809
9.N	4.406078	3.964749	2.028381
10.C	3.271029	4.680012	2.009867
11.H	5.185496	10.009196	3.796973
12.H	5.606542	10.953847	2.348428
13.H	6.525592	8.685370	2.224219
14.H	5.153865	9.805034	0.047122
15.H	3.129526	8.565115	0.660020
16.O	3.700055	7.375525	−0.930897
17.H	5.068802	6.224743	1.110734
18.H	1.432583	7.367994	1.769278
19.H	2.836743	1.066338	2.398500
20.H	5.188863	0.787238	2.217154
21.H	6.163171	2.233204	2.022378
22.P	6.857375	8.349083	−1.626826
23.O	7.687387	9.608549	−1.759749

24.O	5.662946	8.261050	-2.573853
25.O	7.728253	6.993845	-1.853524
26.C	8.842267	6.636702	-0.966979
27.C	1.353022	-3.022082	-0.950589
28.C	9.065911	5.135266	-1.036834
29.O	7.899429	4.451508	-0.474135
30.C	9.280803	4.549687	-2.460121
31.O	10.379837	3.616870	-2.514563
32.C	7.920217	3.889943	-2.796861
33.C	7.451568	3.428811	-1.388065
34.C	-1.958936	-4.224410	2.184866
35.N	6.022115	3.262503	-1.228984
36.C	-1.738847	-2.828415	2.334268
37.H	-2.254289	-4.713748	-1.118712
38.N	0.077080	-3.615439	-0.962369
39.N	1.814962	-5.260692	2.231909
40.H	-1.662325	-6.350574	-1.232660
41.C	-0.167840	-4.971806	-1.118816
42.O	4.848512	-6.973784	-3.422048
43.O	1.468626	-1.776688	-0.821853
44.H	3.092051	-8.007560	-3.507547
45.C	3.977630	7.946437	0.338133
46.N	6.048726	-3.155929	1.836845
47.H	5.316781	-5.294044	-1.219413
48.H	7.178376	-9.726574	-1.261760
49.H	5.376811	-9.482619	-3.202681
50.O	-3.700055	-7.375525	-0.930897
51.C	5.051337	4.264935	-1.210677
52.N	3.832606	3.772842	-1.117882
53.O	2.219582	-0.638060	2.468856
54.C	2.644570	-4.200125	2.191557
55.C	10.109800	-4.987861	2.783669
56.N	2.090647	-2.938864	2.323627
57.C	4.265740	6.897639	1.431461
58.C	2.050641	-5.339647	-1.169391
59.O	-0.641516	-2.227204	2.453703
60.H	-3.077607	-9.782993	2.914563
61.N	-1.064482	-5.292694	2.120980
62.N	3.960693	-4.401331	2.043799
63.C	4.675861	-3.266172	2.034136
64.N	-1.448501	-5.360063	-1.206267
65.O	-10.440010	3.603142	2.526526
66.C	-10.109800	4.987861	2.783669
67.C	-8.841980	5.447769	2.073670
68.O	-7.694912	4.687012	2.604694
69.C	-8.818358	5.238780	0.542800
70.O	-8.117794	6.386351	-0.031150
71.C	-7.951356	3.975773	0.383571
72.C	-6.897912	4.260745	1.472730
73.N	-6.048726	3.155929	1.836845
74.C	-6.356204	1.797650	1.928307
75.N	-5.287926	1.060152	2.155846
76.C	-4.219069	1.954595	2.210528
77.C	-2.821807	1.734971	2.350811
78.O	-2.219582	0.638060	2.468856
79.N	-2.090647	2.938864	2.323627
80.C	-2.644570	4.200125	2.191557
81.N	-1.814962	5.260692	2.231909
82.N	-3.960693	4.401331	2.043799
83.C	-4.675861	3.266172	2.034136
84.H	-9.997506	5.162721	3.861213
85.H	-10.953128	5.582383	2.419219
86.H	-8.687910	6.512271	2.285987
87.H	-9.817015	5.144611	0.110960
88.H	-8.565872	3.123352	0.702514
89.O	-7.382924	3.710219	-0.889453
90.H	-6.227733	5.065890	1.151434
91.H	-7.365137	1.427235	1.814891
92.H	-1.059255	2.833823	2.396071
93.H	-0.782016	5.185759	2.195489
94.H	-2.230151	6.157530	2.010160
95.P	-8.380428	6.859783	-1.567421
96.O	-9.627793	7.710292	-1.685058
97.O	-8.323891	5.663102	-2.513950
98.O	-7.015058	7.709931	-1.812675
99.C	-6.639765	8.829890	-0.941041
100.C	-5.140729	9.055185	-1.046757
101.O	-4.442224	7.897884	-0.483972
102.C	-4.586852	9.253246	-2.485092
103.O	-3.659410	10.354451	-2.574096
104.C	-3.930408	7.890350	-2.818493
105.C	-3.438108	7.440232	-1.413725
106.N	-3.266589	6.013348	-1.240169
107.C	-4.268152	5.042202	-1.203039
108.N	-3.774308	3.825044	-1.102262
109.C	-2.390721	3.982120	-1.078094
110.C	-1.353022	3.022082	-0.950589
111.O	-1.468626	1.776688	-0.821853
112.N	-0.077080	3.615439	-0.962369
113.C	0.167840	4.971806	-1.118816
114.N	1.448501	5.360063	-1.206267
115.N	-0.819326	5.880913	-1.198723
116.C	-2.050641	5.339647	-1.169391
117.H	-6.904774	8.584231	0.089924
118.H	-7.178376	9.726574	-1.261760
119.H	-4.902138	9.939927	-0.443585
120.H	-5.376811	9.482619	-3.202681
121.O	-4.848512	6.973784	-3.422048
122.H	-3.092051	8.007560	-3.507547
123.H	-2.464387	7.899231	-1.197115
124.H	-5.316781	5.294044	-1.219413
125.H	0.720095	2.951702	-0.907689
126.H	2.254289	4.713748	-1.118712
127.H	1.662325	6.350574	-1.232660
128.O	-7.013472	-4.797493	-3.430314
129.H	-8.043508	-3.036955	-3.466685
130.O	10.440010	-3.603142	2.526526
131.H	-7.906217	-2.459426	-1.144979
132.H	-5.304867	-5.312969	-1.235065
133.H	-2.956070	0.720052	-0.893383
134.H	-4.719891	2.256297	-1.086869
135.H	-6.358975	1.664034	-1.188938
136.H	-5.068802	-6.224743	1.110734
137.H	-1.432583	-7.367994	1.769278
138.H	10.284798	2.959678	-1.800044
139.H	-2.836743	-1.066338	2.398500
140.C	-5.051337	-4.264935	-1.210677
141.N	-3.832606	-3.772842	-1.117882
142.C	-3.988602	-2.389177	-1.081044

143.C	-3.027601	-1.352373	-0.950426
144.O	-1.781610	-1.468507	-0.829238
145.N	-5.368398	1.450769	-1.163045
146.N	-5.888500	-0.816621	-1.170564
147.C	-5.346852	-2.047856	-1.156476
148.H	-8.591180	-6.925638	0.056056
149.H	-5.188863	-0.787238	2.217154
150.H	-2.977779	10.263374	-1.882288
151.H	-6.163171	-2.233204	2.022378
152.P	-6.857375	-8.349083	-1.626826
153.O	-7.687387	-9.608549	-1.759749
154.O	-5.662946	-8.261050	-2.573853
155.O	-7.728253	-6.993845	-1.853524
156.C	-8.842267	-6.636702	-0.966979
157.N	-3.620994	-0.076229	-0.948327
158.Na	-10.438888	6.305556	-3.477086
159.C	-9.065911	-5.135266	-1.036834
160.O	-7.899429	-4.451508	-0.474135
161.C	-9.280803	-4.549687	-2.460121
162.C	6.897912	-4.260745	1.472730
163.N	5.287926	-1.060152	2.155846
164.C	4.219069	-1.954595	2.210528
165.H	2.464387	-7.899231	-1.197115
166.C	2.821807	-1.734971	2.350811
167.H	9.997506	-5.162721	3.861213
168.H	10.953128	-5.582383	2.419219
169.H	8.687910	-6.512271	2.285987
170.H	8.565872	-3.123352	0.702514
171.O	7.382924	-3.710219	-0.889453
172.H	6.227733	-5.065890	1.151434
173.H	7.365137	-1.427235	1.814891
174.O	-3.624960	-10.451557	2.463162
175.H	4.902138	-9.939927	-0.443585
176.H	-0.720095	-2.951702	-0.907689
177.H	1.059255	-2.833823	2.396071
178.H	0.782016	-5.185759	2.195489
179.H	2.230151	-6.157530	2.010160
180.P	8.380428	-6.859783	-1.567421
181.O	9.627793	-7.710292	-1.685058
182.O	8.323891	-5.663102	-2.513950
183.N	-2.942367	-2.096739	2.316255
184.O	7.015058	-7.709931	-1.812675
185.C	6.639765	-8.829890	-0.941041
186.C	5.140729	-9.055185	-1.046757
187.O	4.442224	-7.897884	-0.483972
188.C	4.586852	-9.253246	-2.485092
189.O	3.659410	-10.354451	-2.574096
190.C	3.930408	-7.890350	-2.818493
191.O	8.117794	-6.386351	-0.031150
192.C	-5.008407	-10.115760	2.719167
193.N	0.819326	-5.880913	-1.198723
194.C	-5.460770	-8.841850	2.015476
195.O	-4.698304	-7.700323	2.557069
196.C	7.951356	-3.975773	0.383571
197.C	3.438108	-7.440232	-1.413725
198.N	3.266589	-6.013348	-1.240169
199.C	4.268152	-5.042202	-1.203039
200.C	-5.244822	-8.808978	0.485775
201.H	9.817015	-5.144611	0.110960
202.O	-6.385971	-8.097876	-0.088136
203.C	-3.977630	-7.946437	0.338133
204.C	-4.265740	-6.897639	1.431461
205.N	3.774308	-3.825044	-1.102262
206.C	-4.204466	-2.649713	2.186366
207.N	-5.264405	-1.820587	2.240809
208.N	-4.406078	-3.964749	2.028381
209.C	-3.271029	-4.680012	2.009867
210.H	-5.185496	-10.009196	3.796973
211.C	2.390721	-3.982120	-1.078094
212.C	8.841980	-5.447769	2.073670
213.O	7.694912	-4.687012	2.604694
214.N	-3.161197	-6.051746	1.803546
215.C	8.818358	-5.238780	0.542800
216.H	-5.606542	-10.953847	2.348428
217.O	3.624960	10.451557	2.463162
218.H	-6.525592	-8.685370	2.224219
219.C	5.008407	10.115760	2.719167
220.C	5.460770	8.841850	2.015476
221.O	4.698304	7.700323	2.557069
222.H	-5.153865	-9.805034	0.047122
223.C	5.244822	8.808978	0.485775
224.H	-3.129526	-8.565115	0.660020
225.H	2.977779	-10.263374	-1.882288
226.O	6.385971	8.097876	-0.088136
227.C	3.988602	2.389177	-1.081044
228.C	3.027601	1.352373	-0.950426
229.O	1.781610	1.468507	-0.829238
230.N	3.620994	0.076229	-0.948327
231.C	4.978805	-0.170030	-1.091167
232.N	5.368398	-1.450769	-1.163045
233.N	5.888500	0.816621	-1.170564
234.C	5.346852	2.047856	-1.156476
235.H	8.591180	6.925638	0.056056
236.H	9.741428	7.166617	-1.294973
237.H	9.942088	4.908343	-0.416651
238.H	9.521867	5.323360	-3.191473
239.O	7.013472	4.797493	-3.430314
240.H	8.043508	3.036955	-3.466685
241.H	7.906217	2.459426	-1.144979
242.H	5.304867	5.312969	-1.235065
243.H	2.956070	-0.720052	-0.893383
244.H	4.719891	-2.256297	-1.086869
245.H	6.358975	-1.664034	-1.188938
246.O	-10.379837	-3.616870	-2.514563
247.C	-7.920217	-3.889943	-2.796861
248.C	-7.451568	-3.428811	-1.388065
249.C	-4.978805	0.170030	-1.091167
250.H	-9.741428	-7.166617	-1.294973
251.H	-9.942088	-4.908343	-0.416651
252.H	-10.284798	-2.959678	-1.800044
253.C	-1.802532	-6.359649	1.889606
254.H	-7.724127	4.369572	-1.555793
255.N	-6.022115	-3.262503	-1.228984
256.H	6.904774	-8.584231	0.089924
257.H	-9.521867	-5.323360	-3.191473
258.H	9.764835	-3.058474	2.971349
259.H	-9.764835	3.058474	2.971349
260.Na	-6.265643	-10.373979	-3.562554
261.N	3.161197	6.051746	1.803546

262.C	6.356204	−1.797650	1.928307
263.H	3.077607	9.782993	2.914563
264.Na	10.438888	−6.305556	−3.477086
265.H	7.094188	5.669864	−2.981151
266.H	−5.713051	7.061541	−2.959383
267.H	−7.094188	−5.669864	−2.981151
268.H	5.713051	−7.061541	−2.959383
269.H	−4.368747	−7.692971	−1.599804
270.H	7.724127	−4.369572	−1.555793
271.H	4.368747	7.692971	−1.599804
272.Na	6.265643	10.373979	−3.562554
273.K	0.000000	0.000000	0.784802