Supporting Information

for

Understanding Alkali Metal Cation Affinities of Multi-Layer Guanine Quadruplex DNA

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Table S15 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4-K^+–G_4–Na^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

Table S16 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4-K^+–G_4–K^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

Table S17 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4-K^+–G_4–Rb^+–G_4** $^+$ at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

Table S18 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K^+–[ ]** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

Table S19 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K^+–Li^+** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

Table S20 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K^+–Na^+** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

Table S21 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K^+–K^+** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

Table S22 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K^+–Rb^+** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

Table S23 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of the **guanine monomer (G)** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

Table S24 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of the **guanosine dimer (GG)** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

Table S25 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of the **guanosine trimer (GGG)** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

Table S26 Cartesian coordinates (in Å) and ADF total bonding energy (in kcal/mol) of **G_4–K^+–G_4–K^+–G_4–[ ]–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

Table S27 Cartesian coordinates (in Å) and ADF total bonding energy (in kcal/mol) of **G_4–K^+–G_4–K^+–G_4–K^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

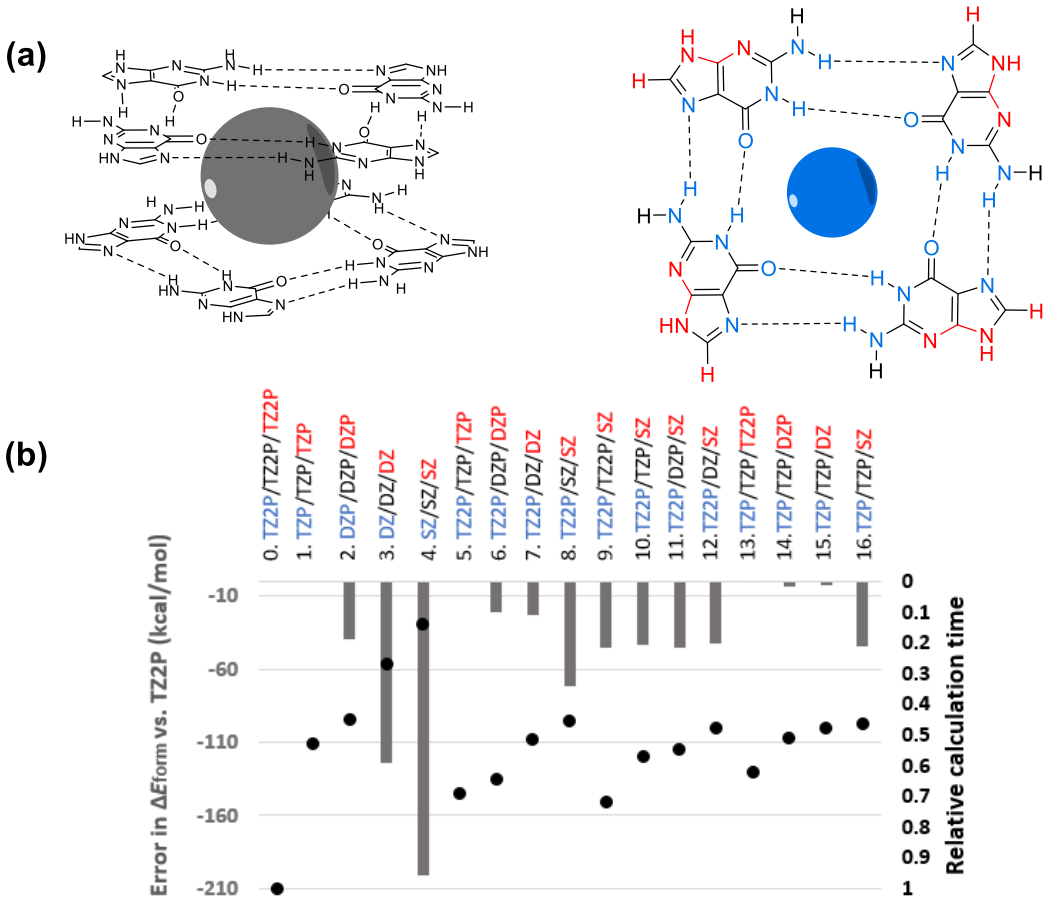

Figure S1 Basis set dependency results for gas phase ZORA-BLYP-D3(BJ) DFT-D calculations on **(a)** G_4–K^+–G_4 using **(b)** different combinations of the basis sets SZ, DZ, DZP, TZP and TZ2P The basis set performance was screened by comparing the calculated formation energy, obtained through stationary point calculations with the specific basis set combination on the optimized double-layer G_4 geometry of Zaccaria *et al.* (Ref. 23), with the TZ2P obtained value. Relative calculation times vs. TZ2P are depicted.

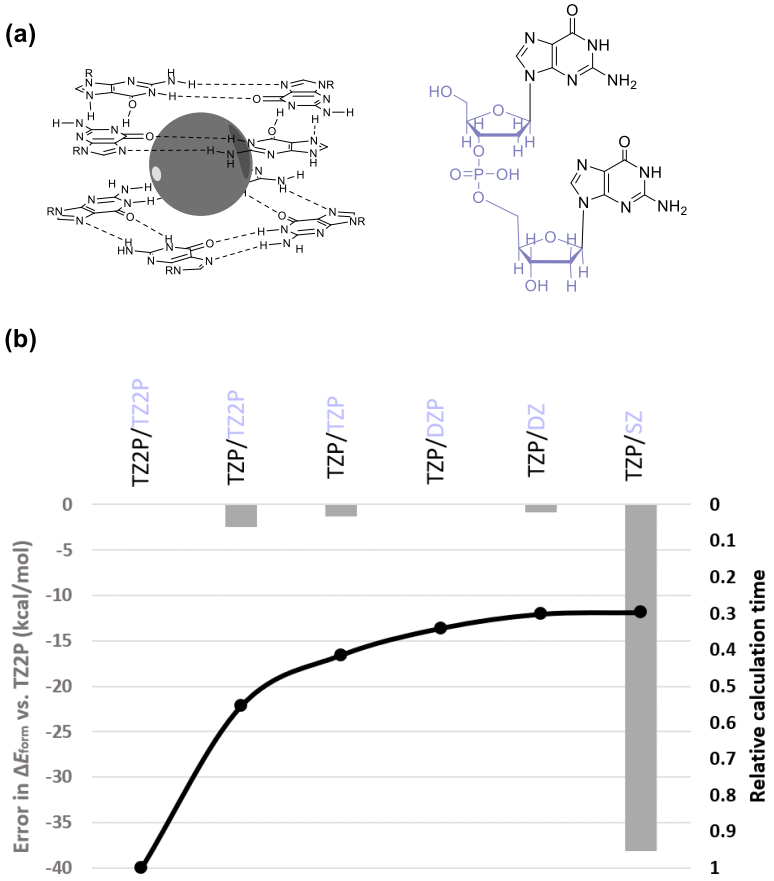

Figure S2 Basis set dependency results for gas phase ZORA-BLYP-D3(BJ) DFT-D calculations on **(a)** GQ–K^+ using **(b)** different combinations of the basis sets SZ, DZ, DZP, TZP and TZ2P The basis set performance was screened by comparing the calculated formation energy, obtained through stationary point calculations on the optimized double-layer GQ geometry at the ZORA-BLYP-D3(BJ)/TZ2P level of theory of Zaccaria *et al.* (Ref. 23), with the TZ2P obtained value. Relative calculation times vs. TZ2P are depicted.

Table S1 Solvation energies (in kcal/mol) and radii (in Å) of alkali metal cations for COSMO computations.

M^+	Experimental ΔG_{hyd} [a]	Ionic Radii Parameter in COSMO[b]	Computed Solvation Energy
Li^+	-113.4	1.4424	-113.5
Na^+	-87.2	1.8685	-87.5
K^+	-70.5	2.3350	-69.8
Rb^+	-65.7	2.4800	-65.6

[a] Marcus, Y. *J. Chem. Soc, Faraday Trans.* **1991**, *87* (18), 2995 –2999.

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

Table S2 Preparation energies (in kcal/mol) of the singly occupied quadruplex structures in the gas phase and solvated state.[a,b]

Structure	M^+	$\Delta E_{prep,gas}$	$\Delta E_{prep,aq}$
G_4–K^+–G_4–**M^+**–G_4	Li^+	9.6	11.9
	Na^+	8.4	10.9
	K^+	4.7	2.0
	Rb^+	5.1	0.3
GQ–K^+–**M^+**	Li^+	9.9	11.4
	Na^+	9.6	12.1
	K^+	5.1	3.1
	Rb^+	4.8	1.2

[a]Energies and geometries computed at the ZORA-BLYP-D3(BJ)/TZP level of theory (G_4 structures) and ZORA-BLYP-D3(BJ)/TZP/DZ level of theory (GQ structures). [b]The solvated state was simulated by using COSMO.

Table S3 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–[ ]–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–[ ]–G_4 (Bond Energy: -19852.70 kcal/mol)			
1.O	-0.215633	-2.309595	1.670163
2.N	-2.513868	-2.578572	1.622327
3.C	-3.663821	-3.349132	1.649219
4.N	-3.648731	-4.691574	1.604228
5.C	-2.401341	-5.210218	1.582677
6.C	-1.180626	-4.517144	1.618026
7.C	-1.197714	-3.093100	1.639539
8.N	-2.050698	-6.547574	1.542787
9.C	-0.666221	-6.614715	1.570452
10.N	-0.110878	-5.413886	1.619343
11.H	-4.956157	-1.680950	1.653059
12.H	-5.671593	-3.278559	1.609748
13.H	-2.582196	-1.536860	1.622797
14.H	-2.690166	-7.337417	1.522591
15.H	-0.138472	-7.559287	1.549035
16.N	-2.711946	4.852088	1.750716
17.O	-2.313889	0.218560	1.669840
18.N	-2.582751	2.516573	1.611205
19.C	-3.353406	3.666679	1.630822
20.N	-4.695745	3.651372	1.582395
21.C	-5.214331	2.403901	1.565206
22.C	-4.521370	1.183329	1.607714
23.C	-3.097361	1.200514	1.632831
24.N	-6.551598	2.053128	1.523899
25.C	-6.618871	0.668786	1.557727
26.N	-5.418173	0.113619	1.611813
27.H	-1.685002	4.958893	1.635096
28.H	-3.282578	5.674347	1.583477
29.H	-1.540975	2.584872	1.614079
30.H	-7.341341	2.692548	1.499125
31.H	-7.563436	0.141006	1.536534
32.N	4.847257	2.713745	1.767993

33.O	0.214154	2.315770	1.661559
34.N	2.512476	2.584545	1.615431
35.C	3.662418	3.355150	1.641149
36.N	3.647401	4.697426	1.592023
37.C	2.400073	5.216067	1.567697
38.C	1.179294	4.523165	1.603977
39.C	1.196312	3.099171	1.629735
40.N	2.049552	6.553329	1.523415
41.C	0.665055	6.620630	1.549653
42.N	0.109611	5.419978	1.601560
43.H	4.954721	1.686971	1.651640
44.H	5.670202	3.284474	1.604026
45.H	2.580772	1.542829	1.619034
46.H	2.689086	7.343063	1.501424
47.H	0.137388	7.565173	1.524934
48.N	2.710395	-4.845450	1.770471
49.O	2.312489	-0.212292	1.670498
50.N	2.581409	-2.510487	1.621210
51.C	3.352012	-3.660482	1.646904
52.N	4.694423	-3.645329	1.600575
53.C	5.213048	-2.397943	1.579182
54.C	4.520013	-1.177239	1.615729
55.C	3.095991	-1.194368	1.638630
56.N	6.550375	-2.047290	1.538462
57.C	6.617561	-0.662833	1.566863
58.N	5.416778	-0.107510	1.616933
59.H	1.683646	-4.952676	1.653739
60.H	3.281343	-5.668355	1.606899
61.H	1.539682	-2.578727	1.622506
62.H	7.340184	-2.686757	1.517327
63.H	7.562130	-0.135090	1.545053
64.N	-4.848790	-2.707337	1.772810
65.N	-2.377419	-5.016430	-1.798573
66.O	1.166423	-2.003618	-1.679887
67.N	-0.549045	-3.555966	-1.652080
68.C	-1.037095	-4.851373	-1.678881
69.N	-0.247908	-5.935263	-1.635902
70.C	1.066376	-5.634010	-1.562518
71.C	1.659489	-4.361053	-1.569373
72.C	0.820488	-3.211035	-1.633029
73.N	2.125063	-6.520374	-1.488484
74.C	3.292705	-5.771814	-1.471718
75.N	3.049097	-4.471007	-1.522709
76.H	-3.057234	-4.247037	-1.637174
77.H	-2.710944	-5.960141	-1.628377
78.H	-1.209946	-2.747067	-1.660828
79.H	2.061550	-7.534780	-1.480203
80.H	4.269899	-6.234848	-1.420808
81.N	-5.012521	2.374478	-1.814765
82.O	-1.999676	-1.168690	-1.679090
83.N	-3.552152	0.546744	-1.659719
84.C	-4.847561	1.034632	-1.690239
85.N	-5.931478	0.245540	-1.645964
86.C	-5.630272	-1.068474	-1.567721
87.C	-4.357283	-1.661550	-1.570783
88.C	-3.207196	-0.822706	-1.635399
89.N	-6.516726	-2.126935	-1.491567
90.C	-5.768148	-3.294495	-1.469805
91.N	-4.467269	-3.051009	-1.519868
92.H	-4.243324	3.054972	-1.655220
93.H	-5.956500	2.708595	-1.647313
94.H	-2.743263	1.207633	-1.669888
95.H	-7.531145	-2.063405	-1.484394
96.H	-6.231240	-4.271544	-1.416353
97.N	2.379261	5.009851	-1.812992
98.O	-1.164650	1.997301	-1.689417
99.N	0.550775	3.549755	-1.664212
100.C	1.038827	4.845103	-1.694175
101.N	0.249573	5.929100	-1.655027
102.C	-1.064765	5.628035	-1.582037
103.C	-1.657838	4.355042	-1.585797
104.C	-0.818763	3.204861	-1.645467
105.N	-2.123551	6.514592	-1.511693
106.C	-3.291188	5.766063	-1.493790
107.N	-3.047492	4.465105	-1.540925
108.H	3.058925	4.240937	-1.648605

109.H	2.712571	5.954051	-1.645049
110.H	1.211681	2.740832	-1.670176
111.H	-2.060073	7.529020	-1.506025
112.H	-4.268448	6.229212	-1.445054
113.N	5.014613	-2.381130	-1.801472
114.O	2.001359	1.162319	-1.683758
115.N	3.553872	-0.552950	-1.655262
116.C	4.849366	-1.040832	-1.681768
117.N	5.933145	-0.251506	-1.638587
118.C	5.631727	1.062762	-1.565460
119.C	4.358698	1.655699	-1.572655
120.C	3.208797	0.816552	-1.636441
121.N	6.517945	2.121593	-1.491604
122.C	5.769233	3.289158	-1.475235
123.N	4.468466	3.045331	-1.526534
124.H	4.245203	-3.061016	-1.640386
125.H	5.958260	-2.714574	-1.630883
126.H	2.745040	-1.213935	-1.663741
127.H	7.532358	2.058204	-1.483041
128.H	6.232114	4.266461	-1.424508

Table S4 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–Li^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory and with COSMO to simulate water.

G_4–Li^+–G_4 (Bond Energy: -19868.96 kcal/mol)			
1.C	3.101792	-4.715586	-1.577707
2.N	0.764965	-3.509914	-1.569008
3.H	-5.104560	1.213396	-1.676938
4.C	4.884632	0.835465	-1.723693
5.N	5.581864	-0.308228	-1.875458
6.H	-4.768539	6.004508	-1.594841
7.C	0.865524	-4.894031	-1.628339
8.N	5.534890	2.008622	-1.716532
9.H	6.262213	-3.920881	-1.522184
10.H	-0.161704	-3.036432	-1.542824
11.H	-1.206392	-5.139291	-1.614002
12.H	-0.198531	-6.599004	-1.612345
13.N	-0.277809	-5.596241	-1.743989
14.N	2.040010	-5.542163	-1.611964
15.C	4.712083	3.070346	-1.631068
16.H	-3.002133	0.168475	-1.561091
17.H	-6.562040	0.204267	-1.709433
18.N	-4.404036	5.055823	-1.580873
19.C	-5.149713	3.890664	-1.576309
20.N	-0.734268	3.487701	-1.546318
21.N	4.434831	-5.077711	-1.547153
22.H	5.132602	-1.235189	-1.710890
23.C	5.180301	-3.912307	-1.543503
24.N	-4.383220	2.812401	-1.575640
25.H	-5.994383	-4.791518	-1.610433
26.H	0.229845	6.577803	-1.586692
27.N	0.310545	5.573943	-1.707941
28.N	-2.008748	5.519829	-1.614197
29.C	-3.070715	4.693357	-1.589140
30.C	-3.070775	3.285610	-1.577900
31.C	-1.822781	2.602446	-1.547574
32.O	-1.624803	1.349894	-1.520786
33.H	6.587720	-0.228142	-1.767314
34.N	3.503747	0.735397	-1.620439
35.H	1.238648	5.117108	-1.576334
36.N	4.413938	-2.834182	-1.563521
37.C	3.101741	-3.307774	-1.579195
38.C	3.915155	5.148435	-1.519657
39.N	2.835686	4.383607	-1.508465
40.C	3.305510	3.071565	-1.572480
41.C	2.621043	1.823988	-1.560882
42.N	-5.045758	-4.427380	-1.585108
43.C	-3.881662	-5.173527	-1.543479
44.N	-2.802742	-4.407939	-1.537158
45.C	-3.274439	-3.095461	-1.574583
46.C	-2.590861	-1.847430	-1.554116
47.H	6.026331	4.765961	-1.622244
48.O	-1.338774	-1.650056	-1.507757
49.N	-3.475089	-0.758612	-1.588327
50.C	-4.857248	-0.858953	-1.681127

51.N	-5.556540	0.284036	-1.818883
52.N	-5.506363	-2.032989	-1.675900
53.O	1.654867	-1.372227	-1.549800
54.C	-0.833969	4.871667	-1.610815
55.H	3.926587	6.229637	-1.475726
56.C	-4.681713	-3.094791	-1.613291
57.H	-3.891699	-6.255281	-1.515587
58.C	1.853444	-2.624859	-1.566515
59.N	5.077795	4.402154	-1.589522
60.O	1.369327	1.627271	-1.503897
61.H	-6.231804	3.899492	-1.569456
62.H	0.192097	3.014119	-1.515312
63.H	4.799569	-6.026420	-1.547538
64.H	3.030705	-0.191596	-1.595841
65.C	5.412450	-1.796803	1.558051
66.N	2.808991	-2.193760	1.611257
67.H	-4.753226	-2.197328	1.618484
68.C	3.251337	3.727201	1.698046
69.N	4.502419	3.213868	1.783528
70.H	-7.592351	1.880998	1.495726
71.C	3.701639	-3.247934	1.695102
72.N	3.092433	5.059915	1.717992
73.H	7.499235	0.701942	1.343718
74.H	1.779419	-2.375186	1.608942
75.H	2.192637	-4.723738	1.665871
76.H	3.860550	-5.251107	1.725907
77.N	3.191941	-4.495576	1.839025
78.N	5.033997	-3.087739	1.675712
79.C	1.799403	5.442096	1.647467
80.H	-2.403329	-1.786756	1.624085
81.H	-5.283908	-3.865083	1.668063
82.N	-6.737335	1.331464	1.484374
83.C	-6.652440	-0.052046	1.433747
84.N	-2.843061	2.218385	1.637775
85.N	6.703833	-1.306170	1.490889
86.H	4.722611	2.217759	1.583902
87.C	6.618620	0.075466	1.404833
88.N	-5.397185	-0.473383	1.464112
89.H	-1.885355	-7.567323	1.590967
90.H	-3.892766	5.279379	1.669956
91.N	-3.227408	4.525030	1.806087
92.N	-5.068082	3.115462	1.651309
93.C	-5.446479	1.822712	1.557341
94.C	-4.623627	0.685209	1.531330
95.C	-3.209652	0.854712	1.587765
96.O	-2.323388	-0.035030	1.601061
97.H	5.254908	3.884237	1.661738
98.N	2.193628	2.837456	1.629461
99.H	-2.223016	4.749537	1.660022
100.N	5.362754	0.496022	1.407286
101.C	4.589011	-0.661192	1.492983
102.C	-0.074790	6.652781	1.572360
103.N	-0.497078	5.397442	1.563512
104.C	0.661063	4.621274	1.600672
105.C	0.829836	3.206195	1.605978
106.N	-1.335711	-6.712627	1.567230
107.C	0.047988	-6.628678	1.521768
108.N	0.469223	-5.373065	1.529615
109.C	-0.689644	-4.598395	1.575918
110.C	-0.859518	-3.183696	1.605128
111.H	1.859392	7.588774	1.654344
112.O	0.030118	-2.297058	1.607542
113.N	-2.223204	-2.816410	1.641017
114.C	-3.280363	-3.707891	1.697131
115.N	-4.531183	-3.196696	1.799003
116.N	-3.120603	-5.040549	1.690554
117.O	2.286383	0.056665	1.503402
118.C	-3.735699	3.275217	1.685141
119.H	-0.701285	7.535196	1.545662
120.C	-1.827319	-5.420656	1.612053
121.H	0.675392	-7.510009	1.483795
122.C	3.174139	-0.830990	1.530666
123.N	1.308865	6.734972	1.620553
124.O	-0.060440	2.320436	1.596451
125.H	-7.532798	-0.679243	1.375774
126.H	-1.813452	2.399042	1.631852

127.H	7.558986	-1.854622	1.523825
128.H	2.372189	1.808293	1.585104
129.Li	0.022435	-0.009859	-1.283306

Table S5 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–Na^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–Na^+–G_4 (Bond Energy: -19861.42 kcal/mol)			
1.O	-0.518620	-2.196057	1.489957
2.N	-2.829065	-2.205539	1.619893
3.C	-4.057902	-2.839355	1.711246
4.N	-4.196035	-4.173892	1.726467
5.C	-3.022468	-4.830929	1.628488
6.C	-1.730639	-4.280940	1.553592
7.C	-1.586277	-2.865189	1.549006
8.N	-2.831767	-6.199452	1.584941
9.C	-1.466799	-6.425572	1.498102
10.N	-0.776726	-5.295892	1.479995
11.H	-5.142482	-1.036009	1.635180
12.H	-6.046344	-2.541342	1.720225
13.H	-2.772225	-1.163591	1.585732
14.H	-3.557707	-6.909927	1.624130
15.H	-1.052081	-7.424402	1.452042
16.N	-2.063947	5.153381	1.827662
17.O	-2.201014	0.514567	1.489920
18.N	-2.210275	2.824722	1.623991
19.C	-2.843702	4.053263	1.719063
20.N	-4.178152	4.191547	1.737715
21.C	-4.835504	3.018329	1.637408
22.C	-4.285853	1.726619	1.558073
23.C	-2.870096	1.582029	1.551602
24.N	-6.204099	2.828048	1.594503
25.C	-6.430617	1.463456	1.503438
26.N	-5.301064	0.773217	1.482133
27.H	-1.041214	5.137791	1.636251
28.H	-2.545474	6.041440	1.728728
29.H	-1.168456	2.767941	1.587073
30.H	-6.914386	3.553976	1.637045
31.H	-7.429560	1.049102	1.456757
32.N	5.149067	2.062361	1.819534
33.O	0.509906	2.198194	1.485733
34.N	2.820287	2.207849	1.616775
35.C	4.048892	2.841737	1.709619
36.N	4.186938	4.176194	1.724653
37.C	3.013492	4.833170	1.624113
38.C	1.721822	4.283110	1.547603
39.C	1.577493	2.867348	1.544658
40.N	2.822810	6.201657	1.578754
41.C	1.458039	6.427638	1.489080
42.N	0.768013	5.297894	1.470988
43.H	5.133235	1.038826	1.632473
44.H	6.037171	2.543450	1.719047
45.H	2.763522	1.165953	1.582937
46.H	3.548668	6.912168	1.618453
47.H	1.043258	7.426309	1.440474
48.N	2.055032	-5.150628	1.833903
49.O	2.191644	-0.512514	1.486079
50.N	2.201045	-2.822483	1.624505
51.C	2.834656	-4.050854	1.721522
52.N	4.169101	-4.189030	1.738421
53.C	4.826285	-3.015971	1.634889
54.C	4.276487	-1.724437	1.553570
55.C	2.860742	-1.579947	1.548878
56.N	6.194821	-2.825677	1.590462
57.C	6.421170	-1.461224	1.496964
58.N	5.291572	-0.771042	1.475358
59.H	1.031949	-5.135687	1.644136
60.H	2.536470	-6.039037	1.737624
61.H	1.159097	-2.765857	1.589377
62.H	6.905137	-3.551529	1.633791
63.H	7.420008	-1.046859	1.448289
64.N	-5.158143	-2.060155	1.819105
65.N	-1.737256	-5.291221	-1.774777
66.O	1.319638	-1.803964	-1.417004

67.N	-0.143685	-3.591664	-1.550285
68.C	-0.438904	-4.942357	-1.655374
69.N	0.503649	-5.898075	-1.675479
70.C	1.758544	-5.409957	-1.609508
71.C	2.157385	-4.062618	-1.548038
72.C	1.156023	-3.053713	-1.501616
73.N	2.936234	-6.133509	-1.590440
74.C	3.980438	-5.225134	-1.528341
75.N	3.549383	-3.974076	-1.502054
76.H	-2.514338	-4.616456	-1.617670
77.H	-1.938083	-6.282033	-1.689695
78.H	-0.906748	-2.883129	-1.504738
79.H	3.021175	-7.145733	-1.627096
80.H	5.015232	-5.541032	-1.503006
81.N	-5.284761	1.742135	-1.770699
82.O	-1.797507	-1.315602	-1.416229
83.N	-3.585199	0.148002	-1.549189
84.C	-4.935762	0.443336	-1.655561
85.N	-5.891184	-0.499341	-1.681304
86.C	-5.402898	-1.754391	-1.619394
87.C	-4.055651	-2.153144	-1.556148
88.C	-3.047079	-1.151758	-1.503555
89.N	-6.126262	-2.932257	-1.606533
90.C	-5.217880	-3.976493	-1.545948
91.N	-3.966943	-3.545329	-1.514910
92.H	-4.610701	2.518663	-1.607958
93.H	-6.275721	1.942266	-1.685216
94.H	-2.876829	0.911153	-1.500300
95.H	-7.138378	-3.017246	-1.645946
96.H	-5.533670	-5.011418	-1.525094
97.N	1.746137	5.287325	-1.784364
98.O	-1.311104	1.801697	-1.411512
99.N	0.152489	3.588577	-1.554319
100.C	0.447714	4.938924	-1.663938
101.N	-0.494714	5.894645	-1.687101
102.C	-1.749568	5.406956	-1.617277
103.C	-2.148400	4.060002	-1.549135
104.C	-1.147098	3.051094	-1.500855
105.N	-2.927149	6.130761	-1.599295
106.C	-3.971297	5.222804	-1.531035
107.N	-3.540330	3.971795	-1.499867
108.H	2.523260	4.613486	-1.623342
109.H	1.946819	6.278517	-1.703113
110.H	0.915615	2.879986	-1.507905
111.H	-3.012025	7.142812	-1.640560
112.H	-5.005996	5.538916	-1.504871
113.N	5.292066	-1.743863	-1.776535
114.O	1.805757	1.314455	-1.418953
115.N	3.593022	-0.149514	-1.552820
116.C	4.943466	-0.445160	-1.659645
117.N	5.899278	0.497180	-1.683982
118.C	5.411436	1.752284	-1.620264
119.C	4.064268	2.151450	-1.557050
120.C	3.055328	1.150310	-1.505867
121.N	6.135219	2.929874	-1.605329
122.C	5.227147	3.974368	-1.543921
123.N	3.976068	3.543561	-1.514100
124.H	4.618341	-2.520641	-1.613495
125.H	6.283153	-1.944142	-1.692634
126.H	2.884441	-0.912555	-1.505203
127.H	7.147367	3.014560	-1.644657
128.H	5.543271	5.009164	-1.521569
129.Na	0.000232	-0.001100	-0.173913

Table S6 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–K^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–K^+–G_4 (Bond Energy: -19863.77 kcal/mol)			
1.O	-0.229529	-2.291954	1.604125
2.N	-2.525148	-2.582919	1.622802
3.C	-3.670978	-3.362559	1.665083
4.N	-3.642508	-4.704768	1.631207
5.C	-2.391887	-5.212888	1.605330
6.C	-1.175474	-4.508097	1.621996

7.C	-1.208488	-3.087659	1.619956
8.N	-2.029225	-6.546091	1.567736
9.C	-0.644015	-6.600710	1.577037
10.N	-0.097602	-5.395542	1.610989
11.H	-4.966536	-1.699871	1.662595
12.H	-5.680624	-3.303142	1.653024
13.H	-2.603547	-1.543902	1.621176
14.H	-2.661567	-7.341955	1.557911
15.H	-0.108436	-7.540846	1.555162
16.N	-2.731299	4.859382	1.767471
17.O	-2.296079	0.232165	1.599237
18.N	-2.587460	2.527698	1.611319
19.C	-3.367396	3.673550	1.648783
20.N	-4.709507	3.644784	1.611139
21.C	-5.217375	2.394019	1.587280
22.C	-4.512470	1.177755	1.608447
23.C	-3.092014	1.210992	1.610443
24.N	-6.550471	2.031079	1.548204
25.C	-6.604935	0.645902	1.561432
26.N	-5.399749	0.099748	1.599081
27.H	-1.704668	4.969151	1.649622
28.H	-3.308181	5.683333	1.633559
29.H	-1.548433	2.605884	1.614339
30.H	-7.346407	2.663275	1.535462
31.H	-7.544962	0.110134	1.539507
32.N	4.854578	2.733256	1.777639
33.O	0.227742	2.297178	1.600769
34.N	2.523233	2.588977	1.615754
35.C	3.668889	3.369052	1.654986
36.N	3.640092	4.711087	1.615461
37.C	2.389349	5.218776	1.587644
38.C	1.173081	4.513792	1.607229
39.C	1.206437	3.093328	1.611886
40.N	2.026410	6.551766	1.545331
41.C	0.641222	6.606154	1.554857
42.N	0.095061	5.401006	1.593454
43.H	4.964615	1.706575	1.660534
44.H	5.678559	3.309920	1.643049
45.H	2.601637	1.549955	1.620111
46.H	2.658526	7.347741	1.532168
47.H	0.105435	7.546083	1.529599
48.N	2.728934	-4.852752	1.785550
49.O	2.293159	-0.226005	1.607334
50.N	2.585109	-2.521438	1.623580
51.C	3.365060	-3.667095	1.664763
52.N	4.707216	-3.638279	1.628730
53.C	5.214919	-2.387527	1.601614
54.C	4.509868	-1.171244	1.619246
55.C	3.089401	-1.204617	1.620451
56.N	6.547988	-2.024589	1.561806
57.C	6.602337	-0.639380	1.570753
58.N	5.397102	-0.093218	1.606672
59.H	1.702420	-4.962816	1.667104
60.H	3.305858	-5.676873	1.653025
61.H	1.546106	-2.600024	1.623754
62.H	7.343984	-2.656730	1.550464
63.H	7.542314	-0.103600	1.547092
64.N	-4.856560	-2.725958	1.784952
65.N	-2.391469	-5.024249	-1.796282
66.O	1.141786	-2.002633	-1.616799
67.N	-0.566093	-3.562916	-1.651208
68.C	-1.052725	-4.860777	-1.687521
69.N	-0.258415	-5.941162	-1.654915
70.C	1.054214	-5.636793	-1.583183
71.C	1.643531	-4.360295	-1.573836
72.C	0.799844	-3.217248	-1.614127
73.N	2.115673	-6.518830	-1.514446
74.C	3.280305	-5.766158	-1.483530
75.N	3.033609	-4.465727	-1.519673
76.H	-3.071218	-4.252931	-1.643159
77.H	-2.727920	-5.971672	-1.656722
78.H	-1.229393	-2.758489	-1.663035
79.H	2.056289	-7.533611	-1.517548
80.H	4.258778	-6.226685	-1.434722
81.N	-5.019407	2.389069	-1.813559
82.O	-1.997652	-1.143546	-1.623607

83.N	-3.558069	0.564141	-1.662234
84.C	-4.855939	1.050579	-1.700924
85.N	-5.936262	0.256316	-1.667151
86.C	-5.631882	-1.056078	-1.591340
87.C	-4.355364	-1.645318	-1.579517
88.C	-3.212316	-0.801693	-1.621825
89.N	-6.513943	-2.117320	-1.520123
90.C	-5.761285	-3.281835	-1.485039
91.N	-4.460844	-3.035250	-1.521196
92.H	-4.248288	3.069069	-1.660440
93.H	-5.966815	2.725701	-1.674316
94.H	-2.753741	1.227561	-1.673529
95.H	-7.528700	-2.057870	-1.522701
96.H	-6.221820	-4.260152	-1.433429
97.N	2.394184	5.017742	-1.811175
98.O	-1.138766	1.995779	-1.630584
99.N	0.568825	3.556400	-1.665436
100.C	1.055313	4.854259	-1.703577
101.N	0.260808	5.934564	-1.673929
102.C	-1.051824	5.630091	-1.602659
103.C	-1.640952	4.353505	-1.591584
104.C	-0.797069	3.210503	-1.629489
105.N	-2.113446	6.512094	-1.536328
106.C	-3.277977	5.759330	-1.504679
107.N	-3.031090	4.458880	-1.538500
108.H	3.073893	4.246893	-1.655679
109.H	2.730259	5.965442	-1.672480
110.H	1.232425	2.752181	-1.672410
111.H	-2.054096	7.526852	-1.539913
112.H	-4.256545	6.219752	-1.457150
113.N	5.021607	-2.395624	-1.797395
114.O	2.000701	1.138453	-1.622323
115.N	3.560621	-0.569748	-1.654816
116.C	4.858389	-1.056712	-1.690910
117.N	5.938938	-0.262514	-1.660192
118.C	5.634849	1.050269	-1.590290
119.C	4.358459	1.639831	-1.581122
120.C	3.215262	0.796329	-1.619719
121.N	6.517106	2.111675	-1.523690
122.C	5.764661	3.276487	-1.494092
123.N	4.464167	3.029990	-1.529116
124.H	4.250305	-3.075250	-1.643651
125.H	5.969049	-2.732038	-1.657953
126.H	2.756252	-1.233122	-1.663388
127.H	7.531858	2.052060	-1.527145
128.H	6.225351	4.254955	-1.447096
129.K	0.000094	0.000076	-0.007972

Table S7 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–Rb^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–Rb^+–G_4 (Bond Energy: -19857.08 kcal/mol)			
1.O	-0.176463	-2.331329	1.773469
2.N	-2.467626	-2.650642	1.697345
3.C	-3.604171	-3.445582	1.678556
4.N	-3.556107	-4.785057	1.600211
5.C	-2.298273	-5.277001	1.592196
6.C	-1.091708	-4.557847	1.660539
7.C	-1.143967	-3.139796	1.719709
8.N	-1.916459	-6.603474	1.529935
9.C	-0.531222	-6.640378	1.574086
10.N	-0.001227	-5.430049	1.655705
11.H	-4.926372	-1.801398	1.689366
12.H	-5.612893	-3.410424	1.609259
13.H	-2.566000	-1.614879	1.742115
14.H	-2.536645	-7.407316	1.480650
15.H	0.016964	-7.572826	1.539249
16.N	-2.831351	4.802769	1.775544
17.O	-2.335651	0.177994	1.767293
18.N	-2.654738	2.469024	1.689187
19.C	-3.449505	3.605661	1.668592
20.N	-4.788887	3.557662	1.588615
21.C	-5.280960	2.299873	1.581183
22.C	-4.562052	1.093282	1.651577

23.C	-3.144049	1.145465	1.711955
24.N	-6.607379	1.918154	1.517490
25.C	-6.644518	0.532954	1.562957
26.N	-5.434355	0.002899	1.646575
27.H	-1.805170	4.927715	1.680524
28.H	-3.414077	5.614364	1.598152
29.H	-1.619077	2.567263	1.735883
30.H	-7.411108	2.538391	1.467029
31.H	-7.576988	-0.015143	1.527249
32.N	4.798996	2.833170	1.782190
33.O	0.174239	2.337247	1.764897
34.N	2.465467	2.656305	1.690828
35.C	3.602101	3.451162	1.672011
36.N	3.554190	4.790468	1.590714
37.C	2.296374	5.282454	1.579956
38.C	1.089696	4.563493	1.648285
39.C	1.141823	3.145569	1.710408
40.N	1.914684	6.608790	1.514363
41.C	0.529387	6.645845	1.556889
42.N	-0.000744	5.435702	1.640338
43.H	4.924162	1.806882	1.688582
44.H	5.610977	3.415746	1.606053
45.H	2.563720	1.620711	1.739058
46.H	2.535008	7.412517	1.464860
47.H	-0.018710	7.578238	1.519275
48.N	2.829212	-4.797369	1.793352
49.O	2.333160	-0.172621	1.771450
50.N	2.652433	-2.463923	1.699609
51.C	3.447360	-3.600510	1.683262
52.N	4.786818	-3.552615	1.604446
53.C	5.278751	-2.294788	1.593366
54.C	4.559622	-1.088080	1.659349
55.C	3.141591	-1.140233	1.719102
56.N	6.605175	-1.913109	1.529653
57.C	6.642100	-0.527770	1.570647
58.N	5.431801	0.002390	1.651604
59.H	1.803144	-4.922528	1.697234
60.H	3.412084	-5.609359	1.618224
61.H	1.616717	-2.562196	1.745296
62.H	7.408975	-2.533447	1.481646
63.H	7.574522	0.020343	1.534045
64.N	-4.801288	-2.827432	1.785758
65.N	-2.487830	-4.987662	-1.788788
66.O	1.123653	-2.052318	-1.788864
67.N	-0.624880	-3.567024	-1.725798
68.C	-1.144578	-4.852808	-1.693092
69.N	-0.376805	-5.949188	-1.609954
70.C	0.943963	-5.675645	-1.560821
71.C	1.565387	-4.415768	-1.617181
72.C	0.751241	-3.256009	-1.718042
73.N	1.983582	-6.579065	-1.453426
74.C	3.166873	-5.854815	-1.463438
75.N	2.953091	-4.551651	-1.562200
76.H	-3.149699	-4.196684	-1.667566
77.H	-2.846530	-5.918139	-1.599433
78.H	-1.270989	-2.751775	-1.782035
79.H	1.899652	-7.591053	-1.407586
80.H	4.133620	-6.337256	-1.396271
81.N	-4.983675	2.485586	-1.798490
82.O	-2.047811	-1.125450	-1.795511
83.N	-3.562868	0.622912	-1.733311
84.C	-4.848778	1.142410	-1.702285
85.N	-5.945135	0.374497	-1.620123
86.C	-5.671386	-0.946186	-1.570065
87.C	-4.411356	-1.567459	-1.625048
88.C	-3.251600	-0.753182	-1.725300
89.N	-6.574771	-1.985898	-1.463273
90.C	-5.850359	-3.169091	-1.472067
91.N	-4.547129	-2.955167	-1.569707
92.H	-4.192777	3.147629	-1.677658
93.H	-5.914367	2.844402	-1.610484
94.H	-2.747725	1.269299	-1.788142
95.H	-7.586766	-1.901963	-1.417648
96.H	-6.332730	-4.135871	-1.404880
97.N	2.490024	4.980946	-1.799153
98.O	-1.121280	2.045184	-1.800352

99.N	0.627132	3.560231	-1.736532
100.C	1.146622	4.846150	-1.705411
101.N	0.378625	5.942612	-1.625667
102.C	-0.942171	5.668973	-1.578009
103.C	-1.563393	4.408940	-1.633328
104.C	-0.748990	3.249036	-1.730903
105.N	-1.982026	6.572468	-1.473561
106.C	-3.165218	5.848123	-1.483990
107.N	-2.951190	4.544831	-1.580509
108.H	3.151819	4.190219	-1.675889
109.H	2.848407	5.911738	-1.610770
110.H	1.273695	2.745037	-1.788896
111.H	-1.898093	7.584457	-1.428054
112.H	-4.132079	6.330601	-1.418734
113.N	4.985171	-2.492323	-1.785854
114.O	2.049947	1.119326	-1.796527
115.N	3.564609	-0.629142	-1.728038
116.C	4.850379	-1.148793	-1.693920
117.N	5.946804	-0.380855	-1.613033
118.C	5.673279	0.940041	-1.567406
119.C	4.413433	1.561363	-1.625549
120.C	3.253619	0.747010	-1.724366
121.N	6.576735	1.979904	-1.462677
122.C	5.852553	3.163189	-1.475880
123.N	4.549390	2.949210	-1.574247
124.H	4.194199	-3.153903	-1.663065
125.H	5.915610	-2.850569	-1.595469
126.H	2.749402	-1.275597	-1.781121
127.H	7.588711	1.896038	-1.416509
128.H	6.335069	4.130055	-1.410939
129.Rb	0.000008	0.000100	-0.008305

Table S8 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–[ ]** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–[ ] (Bond Energy: -36763.39 kcal/mol)			
1.H	10.702103	-1.796939	2.311936
2.H	11.655217	-2.233978	0.855917
3.H	10.440728	-4.204753	1.749256
4.H	10.296926	-3.767494	-0.969451
5.H	8.343594	-2.240148	-0.747314
6.H	7.601217	-3.765506	-1.306207
7.H	6.962175	-4.359688	0.995620
8.P	8.528021	-6.418485	-1.211587
9.O	8.894154	-8.030181	-0.672399
10.O	8.729460	-5.993179	-2.753859
11.O	6.843608	-6.341981	-0.796028
12.C	6.307904	-6.929915	0.516839
13.C	5.245107	-7.991270	0.228509
14.O	3.876455	-7.373340	0.039695
15.C	5.464772	-8.827255	-1.051134
16.O	4.906071	-10.212962	-0.879496
17.C	4.728414	-8.041335	-2.160467
18.C	3.559514	-7.306353	-1.450040
19.H	-7.432337	-5.450600	-2.022033
20.H	-8.799284	-4.352948	-2.332235
21.C	8.165460	-3.291588	-0.497666
22.H	-7.482434	-7.172857	1.627922
23.H	-9.106613	-6.476522	-0.608054
24.H	-7.744105	3.706272	-0.743913
25.C	-2.037236	-10.631817	1.409812
26.C	7.451100	-3.394549	0.865889
27.H	-9.846747	0.848391	1.773885
28.O	1.358700	10.544921	1.168690
29.C	2.552730	10.868969	2.020686
30.C	3.647867	9.812686	1.886740
31.O	3.091647	8.484114	2.390278
32.C	4.112411	9.541847	0.436221
33.O	5.623585	9.270434	0.625086
34.C	3.363791	8.272797	0.014328
35.C	3.354593	7.452035	1.317763
36.H	2.248218	10.955119	3.072051
37.H	2.915445	11.834913	1.654262
38.H	4.510876	10.079184	2.510276

39.H	4.006654	10.392459	-0.241509
40.H	2.342541	8.565059	-0.261759
41.H	3.818943	7.737338	-0.824497
42.H	4.321584	6.981236	1.505435
43.P	6.527219	8.497887	-0.671169
44.O	8.160491	8.757109	-0.134428
45.O	6.089676	8.838180	-2.185300
46.O	6.386285	6.794874	-0.370034
47.C	6.922671	6.179828	0.931017
48.C	7.983354	5.123438	0.618758
49.O	7.357877	3.773850	0.341219
50.C	8.854002	5.397938	-0.626578
51.O	10.224319	4.802921	-0.454204
52.C	8.080965	4.738790	-1.792819
53.C	7.313869	3.543454	-1.165753
54.H	6.050361	5.715831	1.398086
55.H	7.344190	6.974195	1.556101
56.H	8.601568	4.981599	1.513515
57.H	9.045269	6.461817	-0.780055
58.H	7.383971	5.462744	-2.225781
59.H	8.771415	4.400756	-2.575194
60.H	7.795589	2.577412	-1.335721
61.H	-5.495783	7.351631	-2.272494
62.H	-4.455073	8.761273	-2.591925
63.O	-1.091783	-9.896088	0.505487
64.H	-2.636249	7.809724	-1.328151
65.H	-7.025292	4.298857	1.575640
66.H	3.927969	-10.140523	-0.678126
67.H	-5.779018	6.003829	1.352904
68.H	10.128435	3.817669	-0.303692
69.P	-8.547233	6.406949	-0.740805
70.O	-8.839832	8.060840	-0.290292
71.O	-8.873977	5.884159	-2.230384
72.O	-6.843245	6.317396	-0.428925
73.C	-6.256637	6.865664	0.880379
74.H	-8.363397	-9.884821	-0.166684
75.C	-5.220039	7.950314	0.584837
76.O	-3.850913	7.357262	0.331172
77.C	-5.494730	8.814358	-0.664940
78.C	-3.371505	-7.445840	1.127281
79.H	-7.838426	-2.607339	-0.976952
80.H	-1.621894	-10.680260	2.425119
81.H	-2.210471	-11.646897	1.023500
82.H	-4.083788	-10.446878	2.061649
83.H	-2.334551	-8.334447	-0.570470
84.H	-3.903367	-7.598885	-1.010982
85.H	-4.325704	-6.958313	1.328088
86.O	-10.587680	1.322300	1.304619
87.H	-8.614827	-5.077637	1.725979
88.P	-6.528360	-8.525377	-0.691018
89.O	-8.089406	-8.925546	-0.039625
90.O	-6.227206	-8.673387	-2.268531
91.O	-6.423807	-6.856423	-0.225855
92.C	-6.999227	-6.343334	1.101437
93.C	-7.999017	-5.222050	0.829221
94.O	-7.295640	-3.908531	0.592965
95.C	-8.887211	-5.421008	-0.411509
96.O	-10.164271	-4.685716	-0.095993
97.C	-8.118557	-4.734095	-1.560440
98.O	-5.479388	-9.415000	0.405382
99.C	-10.915917	2.547835	2.108595
100.C	-9.855550	3.634223	1.942194
101.O	-8.534535	3.094517	2.482795
102.C	-3.364176	-8.158863	-0.241385
103.C	-7.337231	-3.574444	-0.888948
104.C	-9.568285	4.038043	0.476253
105.H	-3.840638	-10.294637	-0.681528
106.O	-9.305769	5.556679	0.600669
107.C	-8.290272	3.279288	0.102699
108.C	-7.488694	3.323082	1.417535
109.H	-11.012185	2.283362	3.169961
110.C	-3.364288	-9.877498	1.460832
111.O	-3.175851	-8.537651	2.149967
112.C	-3.965626	-9.526730	0.086015
113.H	-11.877551	2.898861	1.720169
114.O	9.924635	-0.999493	0.545370

115.H	-10.126009	4.522887	2.526894
116.C	10.643160	-2.107779	1.262928
117.C	9.880992	-3.436702	1.200312
118.O	8.541755	-3.276782	1.899566
119.H	-10.409685	3.897029	-0.206481
120.C	9.525018	-3.933593	-0.212934
121.H	-8.573616	2.246567	-0.137508
122.H	-10.759488	-4.746278	-0.898010
123.O	9.384782	-5.462975	-0.004388
124.H	5.857524	-6.082818	1.040176
125.H	7.140513	-7.362971	1.081211
126.H	5.157206	-8.634651	1.112557
127.H	6.521933	-8.994461	-1.267997
128.H	5.416152	-7.324431	-2.619147
129.H	4.357178	-8.720450	-2.937723
130.H	2.592033	-7.799134	-1.573829
131.O	-4.939467	10.199605	-0.481655
132.C	-4.795153	8.059976	-1.820134
133.C	-3.597311	7.313595	-1.172533
134.H	-7.068408	7.268188	1.495807
135.H	-5.108051	8.571800	1.481517
136.H	-3.954236	10.129761	-0.316831
137.H	10.375322	-0.832669	-0.328847
138.H	8.474192	9.711029	-0.186914
139.H	-6.139111	-5.955257	1.652207
140.H	-6.560550	8.976696	-0.837247
141.H	-0.185160	-10.297661	0.618131
142.H	0.868502	9.800534	1.615174
143.H	-9.803803	8.344213	-0.334778
144.H	9.861501	-8.292014	-0.757726
145.N	1.285277	5.406714	-1.834188
146.N	-0.989472	5.848056	-1.679126
147.C	-2.207047	5.275691	-1.683190
148.O	2.307615	-0.365667	1.553457
149.H	-1.487385	5.034437	1.469691
150.N	2.474934	-2.673539	1.412452
151.H	-3.050115	5.824917	1.295690
152.C	3.192846	-3.858598	1.335942
153.H	7.558596	-0.526036	1.054845
154.C	-4.447879	1.380795	1.660736
155.N	3.384471	-5.917421	-1.828202
156.N	2.354123	6.417164	1.402336
157.N	-0.191664	3.589705	-1.814338
158.C	0.961040	6.537057	1.365538
159.N	0.363514	5.362035	1.427137
160.C	1.390842	4.419953	1.487961
161.C	1.348911	2.994994	1.520454
162.O	0.333949	2.256309	1.537478
163.N	-0.350490	-5.405322	1.313779
164.C	-1.367644	-4.457910	1.458935
165.N	2.645946	2.428541	1.523928
166.C	-1.323041	-3.036537	1.558646
167.C	3.830020	3.150980	1.539600
168.N	4.997527	2.472928	1.587039
169.N	3.860444	4.496277	1.530392
170.C	2.638717	5.054469	1.485577
171.C	-3.022666	1.345396	1.669163
172.H	-4.826319	2.146803	-1.677406
173.H	-0.500893	-7.545196	1.069725
174.N	-3.633876	-0.170434	-1.702984
175.N	-4.970771	-2.524615	1.810840
176.H	-2.978091	0.638604	-1.771821
177.H	-2.642066	-1.428318	1.677634
178.H	-5.022851	-1.494784	1.716470
179.H	-5.807124	-3.056400	1.543809
180.H	-6.442122	1.441330	-1.512820
181.C	-4.998126	0.040154	-1.586209
182.H	1.432457	-2.692876	1.456043
183.N	-2.461851	2.643544	1.603264
184.H	0.464697	7.496274	1.307366
185.H	2.671021	1.385148	1.519694
186.H	5.040615	1.446849	1.446694
187.H	5.832263	3.002958	1.313126
188.O	-1.774773	-1.532279	-1.922107
189.H	1.487037	-5.074643	1.305544
190.H	3.047071	-5.852577	1.062367

191.N	-2.349488	-6.438625	1.286747
192.H	-5.231667	-5.440031	-1.312462
193.N	-5.886414	-0.960292	-1.458721
194.N	2.520701	-5.029671	1.373239
195.N	4.533426	-3.887715	1.247349
196.C	5.091500	-2.665336	1.237921
197.C	4.368555	-4.925174	-1.898020
198.N	-5.972958	-3.406469	-1.354639
199.C	-4.987131	-4.395246	-1.446138
200.N	3.849423	-3.717984	-2.012036
201.O	-0.309286	-2.294309	1.569276
202.N	5.929851	3.408025	-1.578560
203.C	4.940549	4.398752	-1.584622
204.N	3.732586	3.893451	-1.745841
205.N	-3.787644	-3.885222	-1.650026
206.C	-3.189643	3.824894	1.577382
207.N	-2.516866	4.994474	1.574224
208.N	-4.535168	3.849182	1.575357
209.C	-5.088069	2.624572	1.601076
210.C	3.910479	2.510003	-1.830758
211.C	-3.967744	-2.499106	-1.672094
212.C	2.958540	1.455775	-1.928571
213.O	1.707065	1.550021	-1.999836
214.N	-6.450069	2.331382	1.552573
215.N	3.574890	0.184260	-1.930069
216.C	4.943003	-0.027695	-1.899382
217.N	5.385001	-1.296840	-2.014497
218.N	5.837195	0.968251	-1.780705
219.C	5.269305	2.186431	-1.731392
220.C	-3.803352	-3.192209	1.670473
221.C	6.584670	-0.994073	1.141564
222.N	-2.619153	-2.469906	1.642339
223.N	5.417656	-0.393360	1.300545
224.C	-5.319788	-2.180090	-1.490388
225.O	-2.277562	0.335644	1.718033
226.C	-3.020721	-1.441778	-1.781337
227.C	2.464253	-3.899947	-1.996056
228.C	1.404024	-2.949546	-2.000021
229.O	1.492947	-1.697013	-2.057997
230.N	0.137126	-3.570593	-1.914684
231.C	-0.068564	-4.939021	-1.884827
232.N	-1.343245	-5.385539	-1.928641
233.N	0.935070	-5.831387	-1.844641
234.C	2.152782	-5.260558	-1.884507
235.H	5.189463	5.440213	-1.431827
236.H	2.916127	-0.624046	-1.983501
237.H	4.766056	-2.131914	-2.011972
238.H	6.385817	-1.429075	-1.931860
239.N	-5.386302	0.348786	1.665569
240.N	-3.836353	-4.532189	1.586736
241.C	-2.618921	-5.085771	1.461285
242.H	5.418791	-5.170733	-1.820612
243.H	-0.677572	-2.916997	-1.905564
244.H	-2.174641	-4.773742	-1.809573
245.H	-1.462484	-6.383702	-1.798251
246.N	-5.442193	1.312813	-1.609626
247.H	-5.469204	5.177511	-1.501698
248.H	0.622573	2.937018	-1.860380
249.C	0.013687	4.957838	-1.767015
250.H	2.122351	4.793078	-1.789045
251.H	1.410233	6.405826	-1.718417
252.C	4.467353	-1.417029	1.347661
253.C	-6.564517	0.937862	1.588502
254.H	-7.522569	0.436286	1.570725
255.C	3.046364	-1.377299	1.449261
256.N	-3.436992	5.930418	-1.578410
257.H	-1.419415	2.667214	1.571171
258.C	-4.421418	4.936084	-1.617486
259.N	-3.904332	3.730636	-1.757144
260.C	-2.520154	3.915526	-1.793143
261.C	-1.460174	2.966808	-1.849643
262.N	6.446039	-2.385230	1.098995
263.C	-0.960700	-6.572832	1.202631
264.O	-1.551254	1.714925	-1.914929

Table S9 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–Li⁺** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–Li⁺ (Bond Energy: -36779.96 kcal/mol)			
1.H	10.549427	-1.622191	2.694402
2.H	11.541457	-2.025726	1.254767
3.H	10.359747	-4.032176	2.129548
4.H	10.283334	-3.607732	-0.592695
5.H	8.292592	-2.123740	-0.432881
6.H	7.599530	-3.665714	-1.008835
7.H	6.902879	-4.267619	1.273874
8.P	8.579032	-6.293122	-0.884865
9.O	8.962403	-7.897023	-0.335127
10.O	8.819726	-5.860023	-2.419409
11.O	6.880607	-6.252670	-0.521322
12.C	6.316686	-6.867416	0.767317
13.C	5.265853	-7.927193	0.432903
14.O	3.899823	-7.312316	0.218290
15.C	5.523351	-8.742009	-0.853349
16.O	4.973493	-10.134810	-0.715465
17.C	4.807854	-7.946040	-1.969209
18.C	3.616844	-7.228911	-1.277684
19.H	-7.383027	-5.396157	-1.766529
20.H	-8.742842	-4.297548	-2.104326
21.C	8.129232	-3.177878	-0.185514
22.H	-7.482550	-7.077677	1.890562
23.H	-9.072418	-6.395897	-0.355411
24.H	-7.588352	3.765471	-0.464936
25.C	-1.868800	-10.390460	1.672687
26.C	7.378324	-3.294132	1.157166
27.H	-9.626233	0.832823	2.043957
28.O	1.267643	10.391768	1.409384
29.C	2.442473	10.747405	2.275118
30.C	3.582936	9.741816	2.125872
31.O	3.075502	8.374728	2.575532
32.C	4.083492	9.537862	0.676877
33.O	5.597615	9.300661	0.887747
34.C	3.376319	8.267087	0.193830
35.C	3.372909	7.395306	1.463287
36.H	2.128930	10.797000	3.326236
37.H	2.766119	11.735998	1.933215
38.H	4.422997	10.022529	2.773953
39.H	3.969113	10.409868	0.028321
40.H	2.351859	8.545188	-0.084512
41.H	3.855941	7.778864	-0.659947
42.H	4.347307	6.938293	1.643246
43.P	6.546743	8.561332	-0.395296
44.O	8.161036	8.852537	0.179637
45.O	6.134176	8.904584	-1.915770
46.O	6.435452	6.852982	-0.111940
47.C	6.986315	6.231090	1.179384
48.C	8.046140	5.180757	0.846141
49.O	7.421047	3.833914	0.557553
50.C	8.905758	5.472494	-0.403025
51.O	10.279633	4.881404	-0.247898
52.C	8.126362	4.823845	-1.571000
53.C	7.364417	3.621504	-0.951216
54.H	6.121887	5.759827	1.653376
55.H	7.412687	7.022212	1.805074
56.H	8.672454	5.029875	1.733702
57.H	9.091631	6.538832	-0.546414
58.H	7.426719	5.551537	-1.992913
59.H	8.812468	4.494206	-2.360699
60.H	7.845627	2.657780	-1.134812
61.H	-5.484715	7.393286	-2.122671
62.H	-4.465053	8.803107	-2.501580
63.O	-0.960975	-9.638504	0.743165
64.H	-2.595848	7.883572	-1.288210
65.H	-6.854940	4.353966	1.851916
66.H	3.989679	-10.074313	-0.539482
67.H	-5.633036	6.104380	1.537835
68.H	10.189154	3.893859	-0.109543
69.P	-8.476259	6.442711	-0.452399
70.O	-8.782263	8.087745	0.020065
71.O	-8.853438	5.918126	-1.929197
72.O	-6.759680	6.385100	-0.211450

73.C	-6.129533	6.956215	1.066979
74.H	-8.246725	-9.853176	0.157996
75.C	-5.110058	8.040120	0.714203
76.O	-3.748350	7.449214	0.419891
77.C	-5.435326	8.880960	-0.539487
78.C	-3.296407	-7.251414	1.362780
79.H	-7.791395	-2.538519	-0.759235
80.H	-1.434978	-10.412912	2.681136
81.H	-2.018099	-11.415119	1.302213
82.H	-3.907561	-10.254658	2.360904
83.H	-2.269613	-8.141447	-0.340498
84.H	-3.864786	-7.455600	-0.762258
85.H	-4.256931	-6.780457	1.573539
86.O	-10.370434	1.313851	1.587580
87.H	-8.593973	-4.966745	1.964715
88.P	-6.451499	-8.449581	-0.385627
89.O	-7.994275	-8.887837	0.284337
90.O	-6.157613	-8.612402	-1.963038
91.O	-6.390460	-6.772004	0.055146
92.C	-6.983399	-6.252819	1.371799
93.C	-7.971222	-5.127623	1.075584
94.O	-7.256092	-3.823263	0.826651
95.C	-8.850536	-5.338814	-0.169760
96.O	-10.126717	-4.594554	0.126666
97.C	-8.070276	-4.670416	-1.321455
98.O	-5.363327	-9.289216	0.713083
99.C	-10.701989	2.521365	2.417271
100.C	-9.662843	3.626963	2.246939
101.O	-8.324439	3.104712	2.763519
102.C	-3.296560	-7.987224	0.006204
103.C	-7.290830	-3.504805	-0.659038
104.C	-9.403472	4.048960	0.780881
105.H	-3.720076	-10.141816	-0.389108
106.O	-9.165706	5.570241	0.912859
107.C	-8.115463	3.319679	0.383847
108.C	-7.299777	3.369826	1.689923
109.H	-10.773618	2.239377	3.475948
110.C	-3.216722	-9.675308	1.736545
111.O	-3.055820	-8.318298	2.400059
112.C	-3.853542	-9.365220	0.368191
113.H	-11.676237	2.863675	2.053090
114.O	9.779885	-0.843534	0.913851
115.H	-9.939003	4.505276	2.844389
116.C	10.518987	-1.930755	1.643387
117.C	9.796312	-3.280551	1.562211
118.O	8.433387	-3.154723	2.222574
119.H	-10.251118	3.895883	0.108559
120.C	9.493212	-3.789178	0.141025
121.H	-8.380189	2.283147	0.139385
122.H	-10.715420	-4.660446	-0.679751
123.O	9.378190	-5.320534	0.348931
124.H	5.851622	-6.033355	1.298417
125.H	7.137695	-7.309942	1.340970
126.H	5.158019	-8.585551	1.303546
127.H	6.586910	-8.896405	-1.047538
128.H	5.501761	-7.218748	-2.401428
129.H	4.460560	-8.616782	-2.764538
130.H	2.656416	-7.727523	-1.430593
131.O	-4.884757	10.272807	-0.398699
132.C	-4.772432	8.112330	-1.707014
133.C	-3.547415	7.383831	-1.091374
134.H	-6.920034	7.367695	1.703856
135.H	-4.968154	8.678357	1.594667
136.H	-3.893473	10.213277	-0.270191
137.H	8.457562	9.812313	0.131544
138.H	-6.132449	-5.869198	1.939632
139.H	-6.507720	9.033130	-0.676632
140.H	-0.044879	-10.024075	0.831757
141.H	0.794391	9.632623	1.848996
142.H	-9.752199	8.353835	0.011888
143.H	10.259374	-0.638811	0.063684
144.H	9.932511	-8.149053	-0.419796
145.N	1.326632	5.464283	-1.807296
146.N	-0.945961	5.910407	-1.619848
147.C	-2.164034	5.338124	-1.591543
148.O	2.139168	-0.371511	1.630987

149.H	-1.346495	5.154868	1.516373
150.N	2.382421	-2.676852	1.557403
151.H	-2.924611	5.958594	1.393857
152.C	3.132859	-3.848743	1.522677
153.H	7.420718	-0.422035	1.320878
154.C	-4.210491	1.483623	1.817523
155.N	3.441323	-5.836299	-1.642331
156.N	2.395744	6.335085	1.494256
157.N	-0.148943	3.649390	-1.695123
158.C	1.007024	6.421449	1.391512
159.N	0.436475	5.233088	1.424063
160.C	1.475895	4.310254	1.538795
161.C	1.477361	2.886355	1.580211
162.O	0.473905	2.113697	1.549114
163.N	-0.323775	-5.138374	1.427478
164.C	-1.352324	-4.207765	1.595366
165.N	2.777796	2.361138	1.657598
166.C	-1.351609	-2.785680	1.668878
167.C	3.944606	3.116776	1.723416
168.N	5.120661	2.469691	1.825715
169.N	3.936308	4.460496	1.706074
170.C	2.707129	4.980922	1.596911
171.C	-2.787645	1.487446	1.756354
172.H	-4.776741	2.207849	-1.490686
173.H	-0.427318	-7.283509	1.221641
174.N	-3.583147	-0.109212	-1.484815
175.N	-4.989300	-2.377203	2.054746
176.H	-2.925179	0.698224	-1.557918
177.H	-2.679751	-1.220569	1.817127
178.H	-5.028505	-1.345105	1.948899
179.H	-5.820538	-2.924315	1.801677
180.H	-6.393183	1.503076	-1.336182
181.C	-4.946546	0.103030	-1.365234
182.H	1.342676	-2.701892	1.566775
183.N	-2.265299	2.789810	1.680545
184.H	0.488276	7.366205	1.301304
185.H	2.809075	1.320587	1.657506
186.H	5.152614	1.440697	1.675765
187.H	5.949923	3.013131	1.559536
188.O	-1.727295	-1.471940	-1.710671
189.H	1.452984	-5.055769	1.461317
190.H	3.031815	-5.844569	1.257143
191.N	-2.292832	-6.218674	1.483319
192.H	-5.188426	-5.376402	-1.083150
193.N	-5.835603	-0.896138	-1.231131
194.N	2.487824	-5.028995	1.558201
195.N	4.473879	-3.841856	1.471587
196.C	4.997252	-2.608866	1.461103
197.C	4.424880	-4.842638	-1.689627
198.N	-5.924999	-3.341901	-1.121672
199.C	-4.941744	-4.332476	-1.217500
200.N	3.905634	-3.634661	-1.795048
201.O	-0.351091	-2.008021	1.619613
202.N	5.978003	3.488931	-1.357020
203.C	4.990765	4.481233	-1.380881
204.N	3.783439	3.976813	-1.552085
205.N	-3.741861	-3.824946	-1.427413
206.C	-3.021349	3.958900	1.691152
207.N	-2.373937	5.136193	1.663757
208.N	-4.364056	3.949636	1.742808
209.C	-4.883319	2.715449	1.789679
210.C	3.960115	2.592212	-1.625269
211.C	-3.919685	-2.438183	-1.449003
212.C	3.008081	1.537652	-1.729783
213.O	1.758635	1.630670	-1.816592
214.N	-6.238193	2.397281	1.800309
215.N	3.623328	0.265697	-1.716646
216.C	4.990757	0.053234	-1.675257
217.N	5.433515	-1.215772	-1.781062
218.N	5.884835	1.048717	-1.549245
219.C	5.317366	2.267714	-1.510584
220.C	-3.815607	-3.015084	1.880784
221.C	6.455407	-0.911635	1.384644
222.N	-2.649465	-2.259683	1.799290
223.N	5.271861	-0.334914	1.498326
224.C	-5.270391	-2.116975	-1.262690

225.O	-2.011542	0.485629	1.754256
226.C	-2.971261	-1.381528	-1.564627
227.C	2.520660	-3.817695	-1.795768
228.C	1.460211	-2.866105	-1.795795
229.O	1.549005	-1.614083	-1.834309
230.N	0.192911	-3.489012	-1.729163
231.C	-0.012392	-4.857089	-1.723384
232.N	-1.287155	-5.303038	-1.790056
233.N	0.990427	-5.750779	-1.684108
234.C	2.209195	-5.179651	-1.704565
235.H	5.240176	5.522767	-1.231672
236.H	2.962796	-0.541978	-1.768247
237.H	4.815895	-2.051924	-1.795495
238.H	6.435798	-1.345708	-1.715986
239.N	-5.133574	0.439432	1.859055
240.N	-3.811630	-4.354349	1.810771
241.C	-2.587563	-4.871934	1.649878
242.H	5.474434	-5.087578	-1.602820
243.H	-0.622295	-2.835283	-1.712333
244.H	-2.118663	-4.697402	-1.645512
245.H	-1.406091	-6.304029	-1.681344
246.N	-5.389279	1.376188	-1.379789
247.H	-5.422394	5.241826	-1.349431
248.H	0.666348	2.995799	-1.722490
249.C	0.055642	5.017434	-1.697801
250.H	2.163365	4.857497	-1.702121
251.H	1.450457	6.466342	-1.713642
252.C	4.336811	-1.372640	1.533035
253.C	-6.324590	1.005692	1.835616
254.Li	0.059343	0.050418	1.523562
255.H	-7.271784	0.484295	1.858682
256.N	-3.392864	5.994768	-1.480111
257.C	2.913897	-1.374573	1.581728
258.H	-1.228463	2.818776	1.611045
259.C	-4.376562	4.999043	-1.478463
260.N	-3.860501	3.790983	-1.598067
261.C	-2.477386	3.975574	-1.661923
262.N	6.347347	-2.302389	1.357591
263.C	-0.908039	-6.321199	1.355248
264.C	-1.417225	3.024559	-1.694778
265.O	-1.507076	1.772057	-1.708082

Table S10 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–Na**$^+$ at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–Na$^+$ (Bond Energy: -36769.80 kcal/mol)			
1.H	10.659031	-1.676763	2.780743
2.H	11.592507	-2.153431	1.324159
3.H	10.393321	-4.101623	2.290573
4.H	10.212152	-3.733206	-0.437447
5.H	8.253169	-2.210445	-0.227324
6.H	7.510863	-3.753036	-0.734270
7.H	6.910614	-4.289829	1.595412
8.P	8.472301	-6.385256	-0.621188
9.O	8.815951	-7.986734	-0.041407
10.O	8.703513	-5.991959	-2.167933
11.O	6.781518	-6.285026	-0.232609
12.C	6.209570	-6.897650	1.053338
13.C	5.143937	-7.941435	0.714244
14.O	3.788937	-7.303466	0.493084
15.C	5.394413	-8.760226	-0.571156
16.O	4.821228	-10.144011	-0.436533
17.C	4.696805	-7.951980	-1.689180
18.C	3.504927	-7.232095	-1.003428
19.H	-7.380956	-5.379686	-1.896029
20.H	-8.755242	-4.298599	-2.229473
21.C	8.085461	-3.255717	0.052119
22.H	-7.483045	-7.113581	1.749943
23.H	-9.069320	-6.430582	-0.517659
24.H	-7.693801	3.797756	-0.290780
25.C	-1.958719	-10.517621	1.544648
26.C	7.392296	-3.325718	1.429429
27.H	-9.768835	0.880828	2.188204
28.O	1.317579	10.556038	1.538257

29.C	2.564328	10.910519	2.297130
30.C	3.657676	9.860612	2.108595
31.O	3.141190	8.535788	2.663513
32.C	4.032152	9.573730	0.634944
33.O	5.554603	9.319155	0.726175
34.C	3.271805	8.292257	0.278651
35.C	3.348148	7.491115	1.592412
36.H	2.332936	11.016294	3.365270
37.H	2.890071	11.871665	1.886353
38.H	4.556228	10.140355	2.673443
39.H	3.872816	10.413703	-0.045534
40.H	2.233077	8.570899	0.060541
41.H	3.681880	7.747948	-0.577293
42.H	4.328029	7.029981	1.729714
43.P	6.375157	8.544766	-0.624876
44.O	8.038203	8.848783	-0.219819
45.O	5.812819	8.845424	-2.105409
46.O	6.298989	6.844698	-0.285574
47.C	6.902376	6.274815	1.006465
48.C	7.973421	5.234226	0.677367
49.O	7.367997	3.864891	0.454465
50.C	8.791258	5.499924	-0.605159
51.O	10.181852	4.944465	-0.468760
52.C	7.994519	4.793551	-1.727077
53.C	7.278275	3.597444	-1.044581
54.H	6.061708	5.804327	1.522350
55.H	7.331080	7.093826	1.593960
56.H	8.627858	5.126942	1.550891
57.H	8.948338	6.564407	-0.790406
58.H	7.266550	5.490223	-2.153812
59.H	8.665592	4.451843	-2.524517
60.H	7.774169	2.637840	-1.209437
61.H	-5.479223	7.375458	-1.820369
62.H	-4.443005	8.777524	-2.186106
63.O	-1.021212	-9.738603	0.668532
64.H	-2.600143	7.848082	-0.940332
65.H	-6.960684	4.346910	2.037656
66.H	3.837936	-10.068503	-0.263907
67.H	-5.701407	6.078419	1.820632
68.H	10.117834	3.960466	-0.294691
69.P	-8.503373	6.488141	-0.231852
70.O	-8.776416	8.133683	0.257265
71.O	-8.853608	5.997528	-1.727036
72.O	-6.795236	6.377663	0.054870
73.C	-6.181663	6.937932	1.346587
74.H	-8.289949	-9.837843	-0.053082
75.C	-5.145386	8.013575	1.018249
76.O	-3.784962	7.408712	0.745472
77.C	-5.439045	8.863567	-0.237000
78.C	-3.345617	-7.348766	1.345652
79.H	-7.845407	-2.545288	-0.849535
80.H	-1.547876	-10.589786	2.560328
81.H	-2.112732	-11.523223	1.126885
82.H	-4.011236	-10.384649	2.192170
83.H	-2.284609	-8.171793	-0.369513
84.H	-3.863641	-7.450054	-0.798676
85.H	-4.308503	-6.881659	1.555096
86.O	-10.512154	1.362599	1.730721
87.H	-8.641236	-5.032014	1.829410
88.P	-6.468241	-8.451147	-0.551013
89.O	-8.029604	-8.875952	0.082700
90.O	-6.144948	-8.591300	-2.124792
91.O	-6.392575	-6.781398	-0.082069
92.C	-6.998715	-6.277669	1.234790
93.C	-8.005686	-5.167166	0.945150
94.O	-7.311889	-3.844965	0.726273
95.C	-8.866799	-5.373158	-0.313647
96.O	-10.158281	-4.654211	-0.021140
97.C	-8.084797	-4.673231	-1.445650
98.O	-5.415870	-9.326889	0.554547
99.C	-10.840301	2.570720	2.560767
100.C	-9.784502	3.663630	2.409234
101.O	-8.457544	3.115367	2.927991
102.C	-3.318864	-8.022710	-0.042921
103.C	-7.333020	-3.505854	-0.755470
104.C	-9.509978	4.098490	0.949726

105.H	-3.756596	-10.153018	-0.544743
106.O	-9.250597	5.615149	1.101360
107.C	-8.232418	3.352525	0.551056
108.C	-7.421300	3.372882	1.860789
109.H	-10.929041	2.284972	3.617149
110.C	-3.298770	-9.787548	1.610336
111.O	-3.135060	-8.463738	2.337372
112.C	-3.899137	-9.408729	0.242743
113.H	-11.805509	2.925979	2.185273
114.O	9.853890	-0.932920	1.003088
115.H	-10.052123	4.539074	3.014732
116.C	10.586112	-2.018108	1.742236
117.C	9.825776	-3.349453	1.727981
118.O	8.495623	-3.168922	2.441521
119.H	-10.356199	3.968114	0.270848
120.C	9.451408	-3.884052	0.333358
121.H	-8.513668	2.323873	0.292182
122.H	-10.737775	-4.720396	-0.834171
123.O	9.316149	-5.408064	0.578567
124.H	5.759817	-6.056727	1.587331
125.H	7.024060	-7.354122	1.625477
126.H	5.021674	-8.598209	1.584202
127.H	6.456010	-8.932748	-0.759981
128.H	5.399216	-7.224244	-2.107494
129.H	4.353151	-8.614029	-2.493295
130.H	2.544111	-7.729876	-1.156975
131.O	-4.871553	10.247184	-0.082241
132.C	-4.767202	8.089649	-1.395709
133.C	-3.557295	7.352124	-0.762108
134.H	-6.979481	7.352218	1.972223
135.H	-5.012678	8.645814	1.904480
136.H	-3.883904	10.173560	0.065365
137.H	8.315687	9.813776	-0.277481
138.H	-6.153764	-5.882097	1.803394
139.H	-6.506778	9.031462	-0.390496
140.H	-0.111272	-10.137153	0.762814
141.H	0.871578	9.814011	2.032607
142.H	-9.737089	8.429066	0.223117
143.H	10.290523	-0.792120	0.117331
144.H	9.773754	-8.275489	-0.144705
145.N	1.316805	5.456739	-1.428225
146.N	-0.957950	5.891316	-1.288897
147.C	-2.169158	5.311079	-1.253639
148.O	2.208048	-0.315067	1.671893
149.H	-1.433262	5.101878	1.898979
150.N	2.408953	-2.620832	1.788715
151.H	-2.997925	5.896541	1.771862
152.C	3.138471	-3.801687	1.816168
153.H	7.481371	-0.450690	1.492511
154.C	-4.366992	1.438175	1.966452
155.N	3.330996	-5.838759	-1.371459
156.N	2.362524	6.449301	1.744989
157.N	-0.143868	3.634631	-1.286200
158.C	0.968854	6.553014	1.735317
159.N	0.386419	5.371190	1.799661
160.C	1.423458	4.438730	1.835388
161.C	1.401488	3.014635	1.815868
162.O	0.393293	2.260062	1.783953
163.N	-0.355124	-5.268822	1.538040
164.C	-1.382296	-4.332332	1.682246
165.N	2.702317	2.465539	1.812265
166.C	-1.364466	-2.909939	1.723150
167.C	3.879835	3.202464	1.814846
168.N	5.052876	2.537746	1.824671
169.N	3.892099	4.547573	1.818637
170.C	2.664097	5.089994	1.812379
171.C	-2.943244	1.415739	1.911959
172.H	-4.827881	2.239084	-1.259952
173.H	-0.475850	-7.411741	1.312975
174.N	-3.631353	-0.061780	-1.266710
175.N	-5.009553	-2.449438	2.011209
176.H	-2.972132	0.746764	-1.238327
177.H	-2.688179	-1.321114	1.843143
178.H	-5.057855	-1.416878	1.928403
179.H	-5.841092	-2.987303	1.742613
180.H	-6.457599	1.530248	-1.247935

181.C	-5.003107	0.138143	-1.249899
182.H	1.367550	-2.644438	1.749335
183.N	-2.391977	2.714707	1.942499
184.H	0.459382	7.506186	1.693057
185.H	2.727421	1.424944	1.767320
186.H	5.089288	1.506279	1.715818
187.H	5.877736	3.072161	1.532747
188.O	-1.747629	-1.403948	-1.341339
189.H	1.444404	-5.010514	1.704745
190.H	3.007721	-5.798439	1.575808
191.N	-2.337821	-6.330530	1.534758
192.H	-5.204694	-5.347357	-1.168562
193.N	-5.888566	-0.872364	-1.215688
194.N	2.470420	-4.974026	1.864317
195.N	4.481064	-3.819807	1.807245
196.C	5.028102	-2.595228	1.753681
197.C	4.304884	-4.836633	-1.317957
198.N	-5.960987	-3.318615	-1.192081
199.C	-4.963975	-4.297183	-1.259731
200.N	3.779641	-3.629202	-1.379374
201.O	-0.360308	-2.146878	1.652773
202.N	5.881699	3.425527	-1.400780
203.C	4.878623	4.400833	-1.379483
204.N	3.671606	3.872872	-1.430847
205.N	-3.760079	-3.773991	-1.386102
206.C	-3.127028	3.891690	2.000463
207.N	-2.460705	5.063546	2.034956
208.N	-4.471447	3.905840	2.035765
209.C	-5.016429	2.679478	2.002216
210.C	3.862401	2.489581	-1.471284
211.C	-3.947597	-2.388375	-1.380999
212.C	2.928687	1.420013	-1.388782
213.O	1.673713	1.497575	-1.285979
214.N	-6.377536	2.382184	1.961181
215.N	3.561465	0.161387	-1.399251
216.C	4.931738	-0.032543	-1.479262
217.N	5.380430	-1.298149	-1.567046
218.N	5.814791	0.980293	-1.478526
219.C	5.231923	2.190422	-1.456252
220.C	-3.836165	-3.103021	1.880682
221.C	6.509331	-0.922148	1.583054
222.N	-2.660898	-2.363421	1.831359
223.N	5.333800	-0.322581	1.659841
224.C	-5.311534	-2.085224	-1.262641
225.O	-2.191125	0.408647	1.828519
226.C	-3.006330	-1.322593	-1.341848
227.C	2.397691	-3.818704	-1.461057
228.C	1.325764	-2.886146	-1.396818
229.O	1.401940	-1.631566	-1.273609
230.N	0.068903	-3.516268	-1.450842
231.C	-0.122952	-4.884283	-1.553894
232.N	-1.387318	-5.329221	-1.696611
233.N	0.887885	-5.769294	-1.531467
234.C	2.097395	-5.188818	-1.462788
235.H	5.117812	5.451821	-1.290080
236.H	2.908020	-0.650042	-1.355566
237.H	4.759563	-2.130349	-1.490525
238.H	6.385631	-1.419415	-1.596158
239.N	-5.302553	0.404396	1.920706
240.N	-3.848927	-4.443982	1.815124
241.C	-2.625435	-4.980882	1.698422
242.H	5.352493	-5.079198	-1.199610
243.H	-0.746521	-2.864509	-1.418883
244.H	-2.222465	-4.719866	-1.575654
245.H	-1.508087	-6.335417	-1.692372
246.N	-5.452393	1.406634	-1.269375
247.H	-5.426890	5.204118	-1.019435
248.H	0.667744	2.979293	-1.283523
249.C	0.052308	5.005966	-1.334536
250.H	2.151723	4.835386	-1.435566
251.H	1.436439	6.462094	-1.462930
252.C	4.387672	-1.347871	1.752339
253.C	-6.484472	0.990089	1.906846
254.H	-7.439825	0.483904	1.875439
255.N	-3.400465	5.963726	-1.155055
256.C	2.964453	-1.323908	1.741454

257.H	-1.351783	2.741930	1.881841
258.C	-4.378924	4.963731	-1.137840
259.N	-3.856631	3.756503	-1.231424
260.C	-2.473410	3.943596	-1.297147
261.N	6.383631	-2.312736	1.639545
262.C	-0.949086	-6.445403	1.442747
263.C	-1.404796	3.003756	-1.266568
264.O	-1.484087	1.747288	-1.202142
265.Na	0.089562	-0.052943	0.263544

Table S11 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K⁺** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–K⁺ (Bond Energy: -36773.26 kcal/mol)			
1.H	10.718828	-1.748817	2.660963
2.H	11.652997	-2.214797	1.201638
3.H	10.462113	-4.171181	2.159885
4.H	10.276714	-3.799107	-0.566096
5.H	8.319988	-2.274850	-0.350858
6.H	7.576343	-3.814982	-0.863633
7.H	6.972815	-4.358747	1.461637
8.P	8.514409	-6.457639	-0.725800
9.O	8.875066	-8.055714	-0.146370
10.O	8.707245	-6.072132	-2.279635
11.O	6.833144	-6.359001	-0.299652
12.C	6.291861	-6.952064	1.008263
13.C	5.218585	-7.999520	0.709569
14.O	3.860501	-7.363198	0.503163
15.C	5.443000	-8.841164	-0.565686
16.O	4.870733	-10.221430	-0.396518
17.C	4.725584	-8.051174	-1.684434
18.C	3.551890	-7.311133	-0.988305
19.H	-7.375186	-5.439001	-1.860063
20.H	-8.749600	-4.354748	-2.182339
21.C	8.150373	-3.320834	-0.074607
22.H	-7.469829	-7.195768	1.774467
23.H	-9.060043	-6.495890	-0.481362
24.H	-7.687339	3.777397	-0.314733
25.C	-1.986618	-10.630632	1.592819
26.C	7.456938	-3.395360	1.301955
27.H	-9.802364	0.799396	2.067335
28.O	1.329137	10.535114	1.454261
29.C	2.559186	10.891243	2.239401
30.C	3.657301	9.842107	2.078052
31.O	3.139167	8.521470	2.641244
32.C	4.052534	9.539712	0.613062
33.O	5.574113	9.291260	0.728209
34.C	3.301624	8.250972	0.261958
35.C	3.364692	7.465837	1.586058
36.H	2.304907	11.001068	3.301879
37.H	2.894264	11.850864	1.832381
38.H	4.547161	10.131388	2.651791
39.H	3.898863	10.371046	-0.079234
40.H	2.264402	8.523168	0.028787
41.H	3.724652	7.698330	-0.582272
42.H	4.344586	7.009898	1.740355
43.P	6.417872	8.519235	-0.609766
44.O	8.073419	8.823907	-0.175492
45.O	5.880254	8.822319	-2.098966
46.O	6.336977	6.818802	-0.274765
47.C	6.919082	6.245726	1.025430
48.C	7.989344	5.200475	0.709804
49.O	7.380252	3.834819	0.474868
50.C	8.826554	5.464956	-0.560365
51.O	10.212765	4.903654	-0.405632
52.C	8.042790	4.764380	-1.695168
53.C	7.308872	3.571689	-1.025110
54.H	6.069469	5.778199	1.529030
55.H	7.343789	7.062329	1.619080
56.H	8.630463	5.087675	1.592454
57.H	8.990521	6.529188	-0.741180
58.H	7.325727	5.465775	-2.132445
59.H	8.724090	4.419345	-2.482455
60.H	7.800594	2.609165	-1.185512

61.H	-5.476058	7.393132	-1.755792
62.H	-4.431388	8.798567	-2.082101
63.O	-1.033473	-9.861522	0.724884
64.H	-2.600874	7.831572	-0.847349
65.H	-6.985958	4.285952	2.031390
66.H	3.891416	-10.141058	-0.204528
67.H	-5.727317	6.020539	1.863856
68.H	10.142445	3.919515	-0.234877
69.P	-8.507267	6.470386	-0.209189
70.O	-8.788101	8.103778	0.315063
71.O	-8.840126	6.014667	-1.719365
72.O	-6.802267	6.355506	0.092698
73.C	-6.199734	6.889931	1.400180
74.H	-8.289668	-9.897723	-0.058430
75.C	-5.156023	7.966258	1.100057
76.O	-3.797706	7.359614	0.820332
77.C	-5.439782	8.844400	-0.138086
78.C	-3.343284	-7.450183	1.376334
79.H	-7.832005	-2.610224	-0.795226
80.H	-1.587108	-10.703939	2.612921
81.H	-2.144768	-11.635916	1.175703
82.H	-4.044668	-10.479535	2.218076
83.H	-2.270372	-8.285688	-0.325486
84.H	-3.837841	-7.548994	-0.774081
85.H	-4.304814	-6.975291	1.573659
86.O	-10.532500	1.301638	1.611031
87.H	-8.621152	-5.110019	1.871661
88.P	-6.459136	-8.516437	-0.538914
89.O	-8.028928	-8.935922	0.077329
90.O	-6.123738	-8.643017	-2.111255
91.O	-6.377357	-6.851440	-0.054224
92.C	-6.984010	-6.356747	1.265689
93.C	-7.989110	-5.242578	0.984500
94.O	-7.292497	-3.920833	0.769552
95.C	-8.855308	-5.439900	-0.272146
96.O	-10.144549	-4.720674	0.029552
97.C	-8.076830	-4.734563	-1.403026
98.O	-5.422749	-9.410184	0.567075
99.C	-10.867967	2.487736	2.469670
100.C	-9.814031	3.586809	2.353846
101.O	-8.491728	3.035573	2.880701
102.C	-3.306900	-8.125366	-0.011114
103.C	-7.320638	-3.572092	-0.708972
104.C	-9.520695	4.051145	0.907393
105.H	-3.760849	-10.251721	-0.516209
106.O	-9.267165	5.564929	1.094387
107.C	-8.235726	3.315637	0.511796
108.C	-7.442533	3.314231	1.832510
109.H	-10.963734	2.175120	3.517743
110.C	-3.320958	-9.889031	1.643468
111.O	-3.153787	-8.566184	2.371289
112.C	-3.903707	-9.505672	0.269517
113.H	-11.831037	2.851354	2.096556
114.O	9.909996	-0.999024	0.887020
115.H	-10.093776	4.449029	2.972621
116.C	10.646350	-2.085030	1.620688
117.C	9.890972	-3.419132	1.600801
118.O	8.560767	-3.248560	2.315948
119.H	-10.357012	3.932714	0.214215
120.C	9.516491	-3.950596	0.205047
121.H	-8.511396	2.291147	0.231153
122.H	-10.726903	-4.780504	-0.781925
123.O	9.384070	-5.475109	0.450208
124.H	5.852352	-6.104132	1.539439
125.H	7.119507	-7.399742	1.568373
126.H	5.112153	-8.639780	1.593889
127.H	6.500696	-9.018391	-0.771554
128.H	5.422551	-7.336470	-2.132808
129.H	4.361187	-8.727489	-2.467223
130.H	2.585147	-7.804563	-1.116490
131.O	-4.869976	10.222850	0.049272
132.C	-4.763887	8.094093	-1.309948
133.C	-3.561411	7.336372	-0.685950
134.H	-7.002021	7.297228	2.024617
135.H	-5.023920	8.578446	2.000346
136.H	-3.882961	10.144073	0.198399

137.H	8.352722	9.788402	-0.232751
138.H	-6.138703	-5.966695	1.837590
139.H	-6.506283	9.018153	-0.293897
140.H	-0.126885	-10.264089	0.833694
141.H	0.861521	9.806375	1.948011
142.H	-9.747947	8.400608	0.271236
143.H	10.350690	-0.846481	0.005185
144.H	9.834178	-8.337193	-0.257794
145.N	1.308831	5.437294	-1.421071
146.N	-0.965281	5.878990	-1.256803
147.C	-2.180705	5.305073	-1.240688
148.O	2.300592	-0.363068	1.826136
149.H	-1.445342	5.037540	1.934915
150.N	2.481526	-2.673501	1.818562
151.H	-3.007233	5.834387	1.790784
152.C	3.203124	-3.859723	1.784354
153.H	7.556247	-0.522862	1.401545
154.C	-4.392444	1.375547	1.991384
155.N	3.379523	-5.923597	-1.377542
156.N	2.379882	6.422498	1.740902
157.N	-0.165356	3.621203	-1.382946
158.C	0.986076	6.529629	1.763576
159.N	0.400944	5.349984	1.846112
160.C	1.438287	4.416818	1.861726
161.C	1.412454	2.994688	1.870146
162.O	0.400457	2.243800	1.886006
163.N	-0.337990	-5.395450	1.655839
164.C	-1.363535	-4.454785	1.787487
165.N	2.710076	2.438018	1.833360
166.C	-1.332723	-3.035638	1.875138
167.C	3.890470	3.170296	1.803248
168.N	5.060592	2.500030	1.799904
169.N	3.906786	4.515585	1.790074
170.C	2.680538	5.063413	1.806524
171.C	-2.969884	1.349040	1.980809
172.H	-4.818766	2.176857	-1.296935
173.H	-0.472159	-7.533380	1.390586
174.N	-3.622338	-0.131853	-1.347172
175.N	-4.983405	-2.539248	2.038158
176.H	-2.971942	0.682298	-1.376851
177.H	-2.656408	-1.435482	1.971297
178.H	-5.029033	-1.507118	1.963905
179.H	-5.815560	-3.070732	1.758123
180.H	-6.441127	1.469309	-1.229663
181.C	-4.992040	0.071168	-1.277267
182.H	1.440465	-2.698523	1.850730
183.N	-2.413307	2.647326	1.988937
184.H	0.479954	7.484826	1.730874
185.H	2.740771	1.396452	1.829742
186.H	5.101895	1.468998	1.701479
187.H	5.887394	3.032793	1.509100
188.O	-1.743464	-1.479533	-1.471311
189.H	1.498501	-5.071284	1.737289
190.H	3.057919	-5.856533	1.539241
191.N	-2.330763	-6.439534	1.579458
192.H	-5.196343	-5.413833	-1.118384
193.N	-5.876883	-0.937237	-1.202383
194.N	2.530043	-5.028942	1.836729
195.N	4.544247	-3.885123	1.715315
196.C	5.098781	-2.662550	1.671699
197.C	4.361071	-4.926546	-1.400726
198.N	-5.950543	-3.384866	-1.151739
199.C	-4.955371	-4.365273	-1.227439
200.N	3.842330	-3.719310	-1.511491
201.O	-0.321170	-2.282088	1.877886
202.N	5.916472	3.409253	-1.401885
203.C	4.918174	4.390578	-1.404210
204.N	3.709595	3.871171	-1.497346
205.N	-3.753478	-3.845536	-1.384166
206.C	-3.145372	3.828007	2.015527
207.N	-2.474186	4.996888	2.049417
208.N	-4.490264	3.845171	2.021880
209.C	-5.038661	2.619405	1.994930
210.C	3.896668	2.487121	-1.542308
211.C	-3.942331	-2.460269	-1.391903
212.C	2.955116	1.423568	-1.525857

213.O	1.696923	1.507848	-1.489900
214.N	-6.398511	2.322997	1.933296
215.N	3.579224	0.158947	-1.523430
216.C	4.950318	-0.043562	-1.548034
217.N	5.394546	-1.312501	-1.631180
218.N	5.838513	0.963647	-1.502038
219.C	5.262940	2.178242	-1.485706
220.C	-3.812945	-3.203682	1.934542
221.C	6.583828	-0.990541	1.507040
222.N	-2.629543	-2.475441	1.937860
223.N	5.415019	-0.386967	1.639531
224.C	-5.303208	-2.152657	-1.247888
225.O	-2.218177	0.338368	1.946701
226.C	-3.001302	-1.396594	-1.418400
227.C	2.457780	-3.906152	-1.545873
228.C	1.394488	-2.963832	-1.538499
229.O	1.478014	-1.705174	-1.523908
230.N	0.129689	-3.586377	-1.517036
231.C	-0.073789	-4.957305	-1.523912
232.N	-1.344732	-5.400069	-1.602663
233.N	0.932538	-5.845744	-1.472365
234.C	2.148006	-5.271430	-1.466767
235.H	5.161989	5.439039	-1.299306
236.H	2.927508	-0.655229	-1.532230
237.H	4.777775	-2.148245	-1.586735
238.H	6.399558	-1.438227	-1.615211
239.N	-5.327372	0.340794	1.944171
240.N	-3.834777	-4.543300	1.847142
241.C	-2.612354	-5.090580	1.756225
242.H	5.409204	-5.171606	-1.295238
243.H	-0.684068	-2.934654	-1.517957
244.H	-2.177143	-4.782510	-1.522006
245.H	-1.471722	-6.403520	-1.543505
246.N	-5.437824	1.342437	-1.288363
247.H	-5.437752	5.202089	-0.995836
248.H	0.646490	2.968814	-1.433113
249.C	0.039900	4.992091	-1.352477
250.H	2.141972	4.817185	-1.464492
251.H	1.436086	6.442147	-1.406612
252.C	4.468569	-1.412260	1.730382
253.C	-6.507194	0.929619	1.899423
254.H	-7.463655	0.426355	1.859251
255.N	-3.408698	5.956821	-1.110683
256.C	3.048552	-1.378241	1.801535
257.H	-1.372816	2.678858	1.964325
258.C	-4.391984	4.960441	-1.129906
259.N	-3.876990	3.755217	-1.276993
260.C	-2.493495	3.942251	-1.341511
261.N	6.451297	-2.382471	1.522949
262.C	-0.939872	-6.564818	1.523672
263.C	-1.431662	2.999687	-1.388287
264.O	-1.517392	1.741448	-1.409045
265.K	0.006480	-0.009082	0.214761

Table S12 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–Rb$^+$** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–Rb$^+$ (Bond Energy: -36767.31 kcal/mol)			
1.H	10.742685	-1.747112	2.623810
2.H	11.665553	-2.208277	1.155881
3.H	10.483831	-4.167035	2.125734
4.H	10.287022	-3.805396	-0.599419
5.H	8.333954	-2.274871	-0.380036
6.H	7.586397	-3.815230	-0.888550
7.H	6.988335	-4.354088	1.437784
8.P	8.517547	-6.464992	-0.736808
9.O	8.883513	-8.058987	-0.149374
10.O	8.699794	-6.089001	-2.294218
11.O	6.838828	-6.366975	-0.300378
12.C	6.308369	-6.945196	1.018681
13.C	5.230448	-7.993456	0.740911
14.O	3.872530	-7.356490	0.534867
15.C	5.444404	-8.852633	-0.524289
16.O	4.871656	-10.229706	-0.332686

17.C	4.720290	-8.076965	-1.648707
18.C	3.553864	-7.323327	-0.954399
19.H	-7.411873	-5.436340	-1.828353
20.H	-8.787369	-4.345368	-2.122207
21.C	8.163184	-3.320225	-0.101942
22.H	-7.462925	-7.216656	1.796729
23.H	-9.077371	-6.498676	-0.431913
24.H	-7.689263	3.804191	-0.331560
25.C	-1.987963	-10.649865	1.568176
26.C	7.474269	-3.391973	1.276833
27.H	-9.830873	0.794596	1.992875
28.O	1.329700	10.557129	1.344961
29.C	2.544782	10.924124	2.148256
30.C	3.646723	9.874233	2.021463
31.O	3.123778	8.561634	2.598746
32.C	4.065115	9.548133	0.568299
33.O	5.584613	9.302428	0.712796
34.C	3.320081	8.253186	0.226729
35.C	3.364230	7.489648	1.564161
36.H	2.270911	11.048377	3.204183
37.H	2.887420	11.878241	1.734549
38.H	4.526984	10.175122	2.603939
39.H	3.922302	10.367761	-0.140104
40.H	2.286285	8.521632	-0.025383
41.H	3.755788	7.687704	-0.602477
42.H	4.341913	7.036042	1.738694
43.P	6.452630	8.515305	-0.600376
44.O	8.100065	8.824102	-0.139430
45.O	5.942241	8.801530	-2.102465
46.O	6.363932	6.818951	-0.248525
47.C	6.927405	6.255757	1.063798
48.C	7.992458	5.199346	0.769250
49.O	7.374470	3.837856	0.533566
50.C	8.849159	5.449554	-0.490848
51.O	10.229612	4.881033	-0.313456
52.C	8.076830	4.746701	-1.632046
53.C	7.323292	3.564650	-0.964635
54.H	6.069190	5.799706	1.563218
55.H	7.352735	7.075123	1.653259
56.H	8.620102	5.085993	1.661508
57.H	9.022150	6.511532	-0.676543
58.H	7.371776	5.450195	-2.085160
59.H	8.767085	4.390583	-2.406526
60.H	7.809443	2.597088	-1.111331
61.H	-5.466759	7.431725	-1.712926
62.H	-4.409720	8.832972	-2.016377
63.O	-1.037366	-9.876754	0.700984
64.H	-2.593535	7.836889	-0.783217
65.H	-7.010892	4.285966	2.025824
66.H	3.893579	-10.145651	-0.136059
67.H	-5.750789	6.021570	1.896526
68.H	10.151186	3.898293	-0.138315
69.P	-8.508639	6.500128	-0.197341
70.O	-8.792277	8.125894	0.348395
71.O	-8.828374	6.066491	-1.716775
72.O	-6.806565	6.378480	0.117866
73.C	-6.212309	6.897887	1.434983
74.H	-8.295380	-9.911366	-0.042178
75.C	-5.157580	7.967767	1.151744
76.O	-3.803681	7.352235	0.870607
77.C	-5.428589	8.862688	-0.077311
78.C	-3.343599	-7.469367	1.366288
79.H	-7.841381	-2.613127	-0.739018
80.H	-1.585461	-10.727586	2.586771
81.H	-2.147078	-11.653349	1.147109
82.H	-4.043566	-10.501471	2.201757
83.H	-2.277612	-8.302289	-0.341456
84.H	-3.845648	-7.561344	-0.782699
85.H	-4.303881	-6.993700	1.567360
86.O	-10.551643	1.306018	1.532089
87.H	-8.604637	-5.126797	1.923515
88.P	-6.471566	-8.524835	-0.532770
89.O	-8.037002	-8.948626	0.091596
90.O	-6.145486	-8.643426	-2.107654
91.O	-6.389606	-6.861822	-0.041207
92.C	-6.980096	-6.375282	1.288996

93.C	-7.985067	-5.256479	1.027174
94.O	-7.287650	-3.935431	0.810230
95.C	-8.868495	-5.444227	-0.218744
96.O	-10.152598	-4.725392	0.104864
97.C	-8.104345	-4.733062	-1.355799
98.O	-5.428001	-9.422543	0.563026
99.C	-10.897711	2.480754	2.402030
100.C	-9.844436	3.583055	2.311789
101.O	-8.526873	3.029099	2.847468
102.C	-3.312750	-8.140412	-0.023113
103.C	-7.333550	-3.577921	-0.664875
104.C	-9.534778	4.065718	0.875021
105.H	-3.774002	-10.264484	-0.532483
106.O	-9.281025	5.576384	1.085661
107.C	-8.246307	3.333526	0.484122
108.C	-7.467004	3.316978	1.812853
109.H	-11.004437	2.154731	3.444934
110.C	-3.322339	-9.908861	1.626221
111.O	-3.153165	-8.588353	2.357655
112.C	-3.911005	-9.520518	0.256247
113.H	-11.857173	2.848094	2.023245
114.O	9.917326	-0.995721	0.857807
115.H	-10.133492	4.436901	2.937883
116.C	10.662169	-2.081325	1.583469
117.C	9.909115	-3.416898	1.567780
118.O	8.581376	-3.248300	2.287723
119.H	-10.363483	3.957846	0.171047
120.C	9.529112	-3.951857	0.174938
121.H	-8.520360	2.312565	0.189512
122.H	-10.746645	-4.781271	-0.698403
123.O	9.393761	-5.475008	0.427779
124.H	5.874882	-6.091249	1.545025
125.H	7.140185	-7.388950	1.575722
126.H	5.128084	-8.621330	1.634538
127.H	6.500599	-9.034000	-0.734667
128.H	5.415492	-7.370805	-2.113014
129.H	4.348022	-8.763658	-2.418645
130.H	2.584527	-7.814930	-1.069266
131.O	-4.851023	10.235093	0.129173
132.C	-4.751891	8.121786	-1.254650
133.C	-3.558622	7.346818	-0.633581
134.H	-7.016977	7.307731	2.054688
135.H	-5.023901	8.568158	2.059722
136.H	-3.865119	10.148525	0.281230
137.H	8.383037	9.786711	-0.209184
138.H	-6.127828	-5.991492	1.854656
139.H	-6.493173	9.045205	-0.236535
140.H	-0.130728	-10.280698	0.804215
141.H	0.845744	9.843266	1.844398
142.H	-9.750164	8.427191	0.293442
143.H	10.355507	-0.834461	-0.023677
144.H	9.843539	-8.337937	-0.259167
145.N	1.301198	5.432511	-1.422784
146.N	-0.970213	5.883752	-1.238218
147.C	-2.190321	5.318472	-1.235575
148.O	2.337540	-0.350706	1.947479
149.H	-1.464098	5.027810	1.968388
150.N	2.507552	-2.661154	1.869708
151.H	-3.022540	5.824936	1.808153
152.C	3.223378	-3.849581	1.794881
153.H	7.582321	-0.519949	1.401733
154.C	-4.424778	1.370140	2.019938
155.N	3.383778	-5.940969	-1.362471
156.N	2.376718	6.448885	1.724575
157.N	-0.187811	3.627760	-1.466765
158.C	0.983013	6.560107	1.762653
159.N	0.395465	5.383892	1.874315
160.C	1.431613	4.449404	1.895174
161.C	1.402787	3.028815	1.946325
162.O	0.389910	2.280815	2.004522
163.N	-0.333385	-5.425638	1.693175
164.C	-1.358387	-4.484033	1.823593
165.N	2.698579	2.466551	1.899489
166.C	-1.323365	-3.068652	1.949754
167.C	3.880845	3.194309	1.834567
168.N	5.048564	2.520109	1.829300

169.N	3.899898	4.538952	1.791092
170.C	2.675165	5.090879	1.811845
171.C	-3.003352	1.338970	2.050646
172.H	-4.821820	2.165664	-1.323529
173.H	-0.472400	-7.559209	1.395022
174.N	-3.636003	-0.152589	-1.432111
175.N	-4.974684	-2.556752	2.053862
176.H	-2.990008	0.661354	-1.504137
177.H	-2.647712	-1.464427	2.057620
178.H	-5.022015	-1.524595	1.991478
179.H	-5.807630	-3.085436	1.770242
180.H	-6.438741	1.463482	-1.191470
181.C	-5.000774	0.057546	-1.301951
182.H	1.468801	-2.689176	1.933796
183.N	-2.441026	2.635575	2.046684
184.H	0.479637	7.516241	1.718680
185.H	2.732356	1.426022	1.926562
186.H	5.091506	1.488689	1.744338
187.H	5.876711	3.048593	1.533133
188.O	-1.772293	-1.511978	-1.645856
189.H	1.514540	-5.061650	1.760496
190.H	3.071278	-5.845145	1.536173
191.N	-2.329490	-6.460770	1.572105
192.H	-5.222955	-5.426381	-1.105446
193.N	-5.886517	-0.946161	-1.189102
194.N	2.547013	-5.016771	1.838596
195.N	4.562638	-3.877361	1.696608
196.C	5.121047	-2.655868	1.666833
197.C	4.369323	-4.948845	-1.418082
198.N	-5.968911	-3.394600	-1.126134
199.C	-4.980348	-4.379625	-1.228032
200.N	3.855712	-3.743611	-1.569241
201.O	-0.308863	-2.320231	1.996517
202.N	5.935861	3.410258	-1.362571
203.C	4.943837	4.397837	-1.391893
204.N	3.735605	3.886965	-1.529618
205.N	-3.781724	-3.866164	-1.426407
206.C	-3.168858	3.819500	2.040036
207.N	-2.493358	4.985907	2.071198
208.N	-4.513606	3.840769	2.018708
209.C	-5.066220	2.616334	1.996915
210.C	3.917728	2.502179	-1.577331
211.C	-3.967072	-2.480481	-1.436204
212.C	2.970821	1.445702	-1.628001
213.O	1.713070	1.538223	-1.666096
214.N	-6.425425	2.322871	1.916386
215.N	3.585831	0.175306	-1.602465
216.C	4.955917	-0.036273	-1.564194
217.N	5.394893	-1.308608	-1.626883
218.N	5.847301	0.965085	-1.477818
219.C	5.279230	2.183708	-1.474475
220.C	-3.805907	-3.224970	1.957631
221.C	6.609398	-0.985186	1.513349
222.N	-2.619253	-2.502503	1.996578
223.N	5.445130	-0.379866	1.675580
224.C	-5.320935	-2.165398	-1.247957
225.O	-2.254393	0.325538	2.059541
226.C	-3.025063	-1.422311	-1.525129
227.C	2.470664	-3.927767	-1.597516
228.C	1.412509	-2.982499	-1.648645
229.O	1.502099	-1.725284	-1.705820
230.N	0.143242	-3.597325	-1.597253
231.C	-0.066522	-4.966853	-1.542101
232.N	-1.340310	-5.406297	-1.595502
233.N	0.936028	-5.856582	-1.456058
234.C	2.154642	-5.288131	-1.471134
235.H	5.191680	5.443763	-1.272039
236.H	2.935656	-0.637316	-1.657755
237.H	4.776412	-2.143133	-1.615746
238.H	6.397886	-1.439915	-1.574674
239.N	-5.361046	0.336639	1.969189
240.N	-3.831101	-4.562722	1.844893
241.C	-2.609308	-5.113798	1.763653
242.H	5.416273	-5.195129	-1.303875
243.H	-0.670700	-2.948477	-1.640436
244.H	-2.172562	-4.787076	-1.541831

245.H	-1.470993	-6.406230	-1.498598
246.N	-5.439569	1.331977	-1.293772
247.H	-5.446319	5.228148	-0.973803
248.H	0.621755	2.978559	-1.559957
249.C	0.028070	4.994685	-1.373218
250.H	2.132953	4.813615	-1.483784
251.H	1.435550	6.434390	-1.357933
252.C	4.497168	-1.404407	1.760950
253.C	-6.537947	0.928894	1.897641
254.H	-7.495350	0.428459	1.846695
255.N	-3.413347	5.972348	-1.077293
256.C	3.080707	-1.367295	1.873152
257.H	-1.400891	2.668782	2.052606
258.C	-4.403379	4.983214	-1.123390
259.N	-3.897809	3.780017	-1.314993
260.C	-2.513671	3.962245	-1.382816
261.N	6.471693	-2.377229	1.503422
262.C	-0.937858	-6.590577	1.535335
263.C	-1.460425	3.016908	-1.495139
264.O	-1.556289	1.762444	-1.587103
265.Rb	0.003964	-0.011354	0.185160

Table S13 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–K^+–G_4–[ ]–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–K^+–G_4–[ ]–G_4 (Bond Energy: -29806.97 kcal/mol)			
1.C	-6.613431	-0.599190	3.119493
2.N	-5.331661	-0.916709	3.216819
3.C	-4.653165	0.301846	3.229390
4.C	-3.260337	0.587958	3.319642
5.O	-2.308080	-0.227262	3.412350
6.N	-3.003840	1.977474	3.308528
7.C	-3.979029	2.960300	3.277284
8.N	-3.577678	4.250380	3.382947
9.N	-5.290817	2.691703	3.194692
10.C	-5.562370	1.369587	3.157440
11.C	3.839536	-4.257378	0.025883
12.H	0.463565	-7.793944	-3.232016
13.N	0.728659	-6.812727	-3.230160
14.H	5.349901	5.689332	0.008909
15.N	4.454122	5.209384	0.001711
16.C	3.202273	5.808781	-0.050793
17.C	2.021584	-6.312790	-3.200575
18.H	-7.440221	-1.296358	3.073727
19.H	-1.994017	2.242468	3.340009
20.H	-2.588289	4.547456	3.267595
21.H	-4.288495	4.941290	3.163957
22.N	2.043692	-4.989183	-3.210050
23.H	7.793905	0.463580	-3.231552
24.N	6.812691	0.728654	-3.229635
25.C	6.312746	2.021575	-3.199858
26.N	2.225533	4.917769	-0.056894
27.C	2.322856	2.362212	0.007496
28.N	4.989144	2.043679	-3.209427
29.C	4.602182	0.703529	-3.241121
30.C	3.311292	0.110689	-3.221200
31.O	2.192991	0.694699	-3.199447
32.N	3.371178	-1.298497	-3.221231
33.H	-5.689283	5.349827	0.008595
34.H	3.528460	-3.892362	-3.223226
35.N	-5.209329	4.454057	0.001367
36.H	5.289644	-3.909770	-3.219897
37.H	5.224388	-0.415485	-0.018870
38.N	3.330204	1.373738	0.041899
39.N	4.250406	3.577676	3.383192
40.H	6.518349	0.784374	0.014717
41.C	4.693412	1.632403	0.036626
42.C	2.861298	3.677273	-0.006139
43.O	1.110318	2.028647	-0.011943

44.H	7.702001	-1.252616	3.025832
45.N	6.807107	-0.773348	3.075231
46.C	6.613431	0.599190	3.119493
47.N	5.331661	0.916709	3.216819
48.C	4.541806	-2.040006	-3.267605
49.C	4.653165	-0.301846	3.229390
50.H	-2.886607	6.962675	-3.172383
51.C	-5.808720	3.202208	-0.050991
52.N	-4.917706	2.225473	-0.057055
53.O	-0.227268	2.308059	3.412425
54.C	2.960312	3.979011	3.277446
55.N	4.428858	-3.384001	-3.325406
56.N	1.977493	3.003823	3.308851
57.C	3.260337	-0.587958	3.319642
58.H	6.962627	2.886594	-3.171491
59.C	4.257433	3.839590	0.026213
60.H	2.448047	-1.781990	-3.205003
61.O	2.308080	0.227262	3.412350
62.N	3.003840	-1.977474	3.308528
63.N	2.691722	5.290781	3.194676
64.C	1.369608	5.562332	3.157326
65.N	5.527137	0.578804	-0.011627
66.N	5.762448	-1.480785	-3.283366
67.C	3.979029	-2.960300	3.277284
68.C	5.732044	-0.132673	-3.254956
69.N	3.577678	-4.250380	3.382947
70.N	5.290817	-2.691703	3.194692
71.C	-3.677200	2.861240	-0.006338
72.C	-2.362127	2.322815	0.007529
73.H	-1.252661	-7.701929	3.025419
74.N	-0.773379	-6.807051	3.074900
75.C	0.599167	-6.613374	3.119058
76.N	0.916692	-5.331619	3.216529
77.C	-0.301870	-4.653132	3.229314
78.C	-0.587980	-3.260318	3.319751
79.O	0.227268	-2.308059	3.412425
80.N	-1.977493	-3.003823	3.308851
81.C	-2.960312	-3.979011	3.277446
82.N	-4.250406	-3.577676	3.383192
83.N	-2.691722	-5.290781	3.194676
84.C	-1.369608	-5.562332	3.157326
85.O	-2.028519	1.110278	-0.011586
86.N	-1.373675	3.330196	0.041881
87.C	-1.632358	4.693399	0.036335
88.N	-0.578792	5.527161	-0.012099
89.N	-2.877370	5.201288	0.059421
90.C	-3.839536	4.257378	0.025883
91.C	5.562370	-1.369587	3.157440
92.H	1.296332	-7.440153	3.073127
93.H	-2.242483	-1.993987	3.340256
94.H	-4.547422	-2.588267	3.267879
95.H	-4.941241	-4.288399	3.163695
96.C	0.703536	-4.602221	-3.241478
97.C	0.110702	-3.311336	-3.221265
98.O	0.694709	-2.193033	-3.199435
99.H	6.883840	-3.083533	-0.080521
100.H	0.388564	-2.986043	0.047346
101.H	-0.415526	-5.224519	-0.019097
102.H	-6.883840	3.083533	-0.080521
103.H	-0.388564	2.986043	0.047346
104.H	0.415526	5.224519	-0.019097
105.H	-0.784430	6.518363	0.014296
106.H	-5.349901	-5.689332	0.008909
107.N	-4.454122	-5.209384	0.001711
108.C	-3.202273	-5.808781	-0.050793
109.N	-2.225533	-4.917769	-0.056894
110.C	-2.861298	-3.677273	-0.006139
111.C	-2.322856	-2.362212	0.007496
112.O	-1.110318	-2.028647	-0.011943

113.N	-3.330204	-1.373738	0.041899
114.C	-4.693412	-1.632403	0.036626
115.N	-5.527137	-0.578804	-0.011627
116.N	-5.201324	-2.877402	0.059825
117.C	-4.257433	-3.839590	0.026213
118.H	0.784430	-6.518363	0.014296
119.H	7.440221	1.296358	3.073727
120.H	1.994017	-2.242468	3.340009
121.H	2.588289	-4.547456	3.267595
122.H	4.288495	-4.941290	3.163957
123.N	-1.298484	-3.371228	-3.221108
124.C	-2.039996	-4.541846	-3.267573
125.H	-3.083610	-6.883905	-0.080346
126.H	-2.986014	-0.388644	0.047423
127.H	-5.224388	0.415485	-0.018870
128.H	-6.518349	-0.784374	0.014717
129.N	-3.384004	-4.428883	-3.325284
130.N	-1.480787	-5.762484	-3.283520
131.C	-0.132669	-5.732088	-3.255274
132.H	-0.463565	7.793944	-3.232016
133.N	-0.728659	6.812727	-3.230160
134.C	-2.021584	6.312790	-3.200575
135.N	-2.043692	4.989183	-3.210050
136.C	-0.703536	4.602221	-3.241478
137.C	-0.110702	3.311336	-3.221265
138.O	-0.694709	2.193033	-3.199435
139.H	-7.793905	-0.463580	-3.231552
140.N	-6.812691	-0.728654	-3.229635
141.C	-6.312746	-2.021575	-3.199858
142.N	-4.989144	-2.043679	-3.209427
143.C	-4.602182	-0.703529	-3.241121
144.C	-3.311292	-0.110689	-3.221200
145.O	-2.192991	-0.694699	-3.199447
146.N	-3.371178	1.298497	-3.221231
147.C	-4.541806	2.040006	-3.267605
148.N	-4.428858	3.384001	-3.325406
149.N	-5.762448	1.480785	-3.283366
150.C	-5.732044	0.132673	-3.254956
151.N	1.298484	3.371228	-3.221108
152.N	-6.807107	0.773348	3.075231
153.C	-0.599167	6.613374	3.119058
154.C	0.132669	5.732088	-3.255274
155.N	5.201324	2.877402	0.059825
156.K	0.000000	0.000000	-1.547723
157.H	2.886607	-6.962675	-3.172383
158.H	-6.962627	-2.886594	-3.171491
159.H	-2.448047	1.781990	-3.205003
160.H	-3.528460	3.892362	-3.223226
161.H	-5.289644	3.909770	-3.219897
162.H	3.909762	5.289659	-3.219766
163.H	1.781981	2.448107	-3.204790
164.H	-1.781981	-2.448107	-3.204790
165.H	-3.909762	-5.289659	-3.219766
166.H	-3.892329	-3.528493	-3.222908
167.H	1.252661	7.701929	3.025419
168.H	5.689283	-5.349827	0.008595
169.N	5.209329	-4.454057	0.001367
170.C	5.808720	-3.202208	-0.050991
171.C	2.039996	4.541846	-3.267573
172.N	3.384004	4.428883	-3.325284
173.N	1.480787	5.762484	-3.283520
174.H	-1.296332	7.440153	3.073127
175.N	4.917706	-2.225473	-0.057055
176.C	3.677200	-2.861240	-0.006338
177.H	2.986014	0.388644	0.047423
178.H	2.242483	1.993987	3.340256
179.H	4.547422	2.588267	3.267879
180.H	4.941241	4.288399	3.163695
181.C	2.362127	-2.322815	0.007529

182.O	2.028519	-1.110278	-0.011586
183.N	0.773379	6.807051	3.074900
184.H	3.892329	3.528493	-3.222908
185.H	3.083610	6.883905	-0.080346
186.N	1.373675	-3.330196	0.041881
187.C	1.632358	-4.693399	0.036335
188.H	-7.702001	1.252616	3.025832
189.N	-0.916692	5.331619	3.216529
190.C	0.301870	4.653132	3.229314
191.C	0.587980	3.260318	3.319751
192.N	0.578792	-5.527161	-0.012099
193.N	2.877370	-5.201288	0.059421

Table S14 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–K^+–G_4–Li^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–K^+–G_4–Li^+–G_4 (Bond Energy: -29826.51 kcal/mol)			
1.C	-6.466789	-0.721246	3.309981
2.N	-5.169413	-0.979309	3.281280
3.C	-4.539080	0.264206	3.290093
4.C	-3.163301	0.623945	3.248007
5.O	-2.159015	-0.150536	3.207590
6.N	-2.979278	2.015104	3.259279
7.C	-4.001986	2.952884	3.331089
8.N	-3.653556	4.251177	3.388187
9.N	-5.300214	2.616984	3.368741
10.C	-5.505098	1.288238	3.333265
11.C	3.205485	-4.755315	0.118738
12.H	0.806766	-7.841919	-3.072511
13.N	1.024179	-6.849057	-3.078078
14.H	5.990497	4.895575	-0.032467
15.N	5.040101	4.536044	-0.014724
16.C	3.875526	5.293404	-0.020267
17.C	2.291945	-6.287985	-3.090679
18.H	-7.259811	-1.457779	3.306748
19.H	-1.980530	2.306375	3.218949
20.H	-2.665139	4.559492	3.260919
21.H	-4.406548	4.924729	3.300600
22.N	2.251062	-4.965269	-3.112350
23.H	7.722596	0.772738	-3.145345
24.N	6.729721	0.990168	-3.147251
25.C	6.168573	2.257753	-3.170358
26.N	2.792319	4.535333	0.015747
27.C	2.559952	1.988875	0.101908
28.N	4.845755	2.216741	-3.182775
29.C	4.523170	0.858562	-3.162666
30.C	3.262275	0.203668	-3.123247
31.O	2.116863	0.731475	-3.099725
32.N	3.390076	-1.200533	-3.095118
33.H	-4.984794	5.985710	-0.042236
34.H	3.670653	-3.783512	-3.117191
35.N	-4.625263	5.035440	-0.018125
36.H	5.427149	-3.717413	-3.101177
37.H	5.080723	-1.137513	0.113283
38.N	3.432000	0.880754	0.137952
39.N	4.222951	3.603769	3.393305
40.H	6.517444	-0.113535	0.061666
41.C	4.817030	0.962614	0.105835
42.C	3.262743	3.222932	0.047946
43.O	1.314140	1.812519	0.118171
44.H	7.559756	-1.100783	3.393480
45.N	6.644006	-0.661701	3.353767
46.C	6.387442	0.696013	3.289319
47.N	5.090004	0.953123	3.255294
48.C	4.594365	-1.886426	-3.142545
49.C	4.459861	-0.289952	3.292450
50.H	-3.272635	6.742536	-3.226597

51.C	-5.382744	3.871244	0.006011
52.N	-4.624298	2.788422	0.047063
53.O	-0.175964	2.105837	3.178107
54.C	2.925645	3.951073	3.313374
55.N	4.544856	-3.232770	-3.226999
56.N	1.988770	2.927153	3.245623
57.C	3.084125	-0.650693	3.259217
58.H	6.776604	3.153150	-3.173795
59.C	4.668412	3.204133	0.033965
60.H	2.491795	-1.728768	-3.075018
61.O	2.079643	0.122667	3.203092
62.N	2.900345	-2.041224	3.300957
63.N	2.589376	5.249703	3.325172
64.C	1.261266	5.453755	3.268644
65.N	5.509578	-0.190379	0.128435
66.N	5.787188	-1.268912	-3.145209
67.C	3.923293	-2.977047	3.393646
68.C	5.692015	0.077684	-3.148485
69.N	3.575094	-4.273801	3.478600
70.N	5.221433	-2.640153	3.424285
71.C	-3.311531	3.258795	0.051917
72.C	-2.076830	2.556471	0.098299
73.H	-1.128447	-7.612141	3.448479
74.N	-0.688966	-6.696764	3.404991
75.C	0.669282	-6.440681	3.350576
76.N	0.926737	-5.143588	3.307575
77.C	-0.316613	-4.513206	3.328194
78.C	-0.676998	-3.137806	3.279971
79.O	0.096809	-2.133841	3.221785
80.N	-2.067884	-2.953718	3.308135
81.C	-3.004540	-3.975874	3.401592
82.N	-4.301828	-3.627054	3.472789
83.N	-2.667949	-5.273727	3.445652
84.C	-1.339863	-5.478848	3.393417
85.O	-1.900162	1.310956	0.130081
86.N	-0.968384	3.428829	0.105958
87.C	-1.050615	4.813173	0.054076
88.N	0.102712	5.505618	0.049925
89.N	-2.218111	5.476539	0.017262
90.C	-3.292830	4.664185	0.016282
91.C	5.426062	-1.312600	3.358626
92.H	1.405795	-7.233689	3.343702
93.H	-2.359772	-1.955326	3.264887
94.H	-4.612092	-2.639084	3.347240
95.H	-4.976746	-4.380679	3.403908
96.C	0.892770	-4.642721	-3.109734
97.C	0.237631	-3.381614	-3.086258
98.O	0.765372	-2.236202	-3.064950
99.H	6.377323	-3.982787	0.080600
100.H	-0.051251	-3.049093	0.200475
101.H	-1.136931	-5.167984	0.145319
102.H	-6.464731	3.891269	-0.006568
103.H	-0.036182	2.960148	0.136338
104.H	1.049725	5.076768	0.030914
105.H	0.025120	6.512526	-0.029171
106.H	-6.077096	-4.987577	0.086500
107.N	-5.126726	-4.627613	0.091749
108.C	-3.962037	-5.384660	0.102511
109.N	-2.878949	-4.625714	0.118771
110.C	-3.349607	-3.313038	0.120401
111.C	-2.646933	-2.077949	0.145697
112.O	-1.401140	-1.901029	0.155847
113.N	-3.519250	-0.969484	0.159129
114.C	-4.904323	-1.052373	0.131265
115.N	-5.597182	0.100719	0.130677
116.N	-5.567847	-2.220285	0.114522
117.C	-4.755296	-3.294888	0.108616
118.H	-0.112045	-6.604732	0.118457
119.H	7.180326	1.432421	3.269049

120.H	1.901664	-2.333500	3.267505
121.H	2.586562	-4.585011	3.359754
122.H	4.328284	-4.948970	3.406705
123.N	-1.166795	-3.509161	-3.072600
124.C	-1.852170	-4.713699	-3.120516
125.H	-3.981880	-6.466706	0.099853
126.H	-3.049987	-0.037150	0.175163
127.H	-5.168494	1.047281	0.092673
128.H	-6.605108	0.022191	0.067076
129.N	-3.197545	-4.664581	-3.222003
130.N	-1.234851	-5.906505	-3.108120
131.C	0.111734	-5.811441	-3.096549
132.H	-0.891943	7.688217	-3.240876
133.N	-1.109480	6.695476	-3.225491
134.C	-2.377339	6.134356	-3.224423
135.N	-2.336569	4.811511	-3.216713
136.C	-0.978295	4.488944	-3.208256
137.C	-0.323187	3.228701	-3.156038
138.O	-0.850922	2.084101	-3.107581
139.H	-7.808092	-0.925592	-3.120394
140.N	-6.815212	-1.142969	-3.119145
141.C	-6.253930	-2.410714	-3.116030
142.N	-4.931115	-2.369863	-3.130560
143.C	-4.608712	-1.011517	-3.139554
144.C	-3.347807	-0.355877	-3.116152
145.O	-2.202355	-0.883083	-3.083762
146.N	-3.475737	1.048598	-3.117545
147.C	-4.680162	1.733243	-3.178499
148.N	-4.630730	3.077426	-3.292788
149.N	-5.872926	1.115785	-3.166184
150.C	-5.777624	-0.230578	-3.140552
151.N	1.081272	3.356406	-3.147094
152.N	-6.723147	0.637596	3.343806
153.C	-0.747767	6.414705	3.205111
154.C	-0.197187	5.657613	-3.221670
155.Li	-0.039736	-0.017054	2.934520
156.K	-0.043178	-0.059803	-1.426585
157.H	3.187324	-6.895990	-3.080126
158.H	-6.861943	-3.305992	-3.100240
159.H	-2.577466	1.577148	-3.109420
160.H	-3.756363	3.630310	-3.195659
161.H	-5.512815	3.564789	-3.176283
162.H	3.598026	5.392046	-3.218189
163.H	1.609457	2.458264	-3.120989
164.H	-1.695035	-2.610762	-3.066685
165.H	-3.683528	-5.545839	-3.093776
166.H	-3.748993	-3.789881	-3.119841
167.H	1.050205	7.587802	3.272903
168.H	4.897686	-6.077667	0.090265
169.N	4.538000	-5.127189	0.093645
170.C	5.295339	-3.962635	0.091718
171.C	1.766662	4.559507	-3.222683
172.N	3.111890	4.508052	-3.325322
173.N	1.149395	5.752357	-3.236070
174.H	-1.484177	7.207440	3.179848
175.N	4.536786	-2.879273	0.107560
176.C	3.224045	-3.349547	0.122178
177.H	2.962640	-0.050943	0.174132
178.H	2.280462	1.927948	3.224390
179.H	4.532816	2.613267	3.287740
180.H	4.897771	4.355378	3.303619
181.C	1.989297	-2.646418	0.152717
182.O	1.812696	-1.400502	0.156293
183.N	0.610594	6.671702	3.251222
184.H	3.663625	3.636021	-3.203543
185.H	3.895626	6.375063	-0.049221
186.N	0.880889	-3.518449	0.180060
187.C	0.963268	-4.903676	0.160577
188.H	-7.638824	1.077557	3.374411

189.N	-1.005518	5.116994	3.193884
190.C	0.237773	4.487035	3.227737
191.C	0.597923	3.110799	3.212634
192.N	-0.189861	-5.596269	0.173724
193.N	2.130855	-5.567571	0.138167
194.N	5.480707	2.129750	0.062704

Table S15 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–K^+–G_4–Na^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–K^+–G_4–Na^+–G_4 (Bond Energy: -29817.37 kcal/mol)			
1.C	-6.514331	-0.908473	3.281674
2.N	-5.213123	-1.148724	3.248398
3.C	-4.604746	0.105978	3.277047
4.C	-3.234754	0.480459	3.219118
5.O	-2.226734	-0.279073	3.143369
6.N	-3.063172	1.876737	3.247822
7.C	-4.095121	2.801010	3.329006
8.N	-3.762071	4.105038	3.377821
9.N	-5.390414	2.449741	3.374018
10.C	-5.581702	1.116833	3.333443
11.C	3.244566	-4.660321	-0.002233
12.H	0.814839	-7.791513	-3.222604
13.N	1.033582	-6.798943	-3.212127
14.H	5.894854	4.967829	-0.082421
15.N	4.954671	4.583721	-0.044485
16.C	3.772687	5.309121	-0.004180
17.C	2.302253	-6.239267	-3.229088
18.H	-7.298157	-1.654766	3.269760
19.H	-2.070241	2.191827	3.206485
20.H	-2.784632	4.450344	3.278403
21.H	-4.526763	4.769397	3.334068
22.N	2.263553	-4.916427	-3.227154
23.H	7.745858	0.820622	-3.229943
24.N	6.753242	1.039141	-3.217950
25.C	6.193455	2.307818	-3.229951
26.N	2.711522	4.522641	0.057175
27.C	2.551412	1.967986	0.136137
28.N	4.870622	2.269016	-3.226557
29.C	4.546769	0.911028	-3.207567
30.C	3.286891	0.258192	-3.154209
31.O	2.142531	0.789446	-3.109980
32.N	3.410794	-1.146142	-3.135778
33.H	-5.008483	5.893194	-0.063512
34.H	3.684068	-3.732623	-3.208194
35.N	-4.624303	4.952956	-0.027746
36.H	5.444274	-3.669646	-3.219559
37.H	5.135090	-1.075369	0.065824
38.N	3.451726	0.887858	0.125457
39.N	4.112985	3.726016	3.363251
40.H	6.561215	-0.022894	-0.018697
41.C	4.835058	1.008691	0.063026
42.C	3.213160	3.221360	0.056697
43.O	1.306924	1.752827	0.212416
44.H	7.684583	-0.917079	3.342212
45.N	6.761859	-0.491984	3.311346
46.C	6.485336	0.864314	3.260824
47.N	5.183984	1.104556	3.232392
48.C	4.613661	-1.834739	-3.203182
49.C	4.575814	-0.150270	3.260853
50.H	-3.247767	6.809057	-3.220320
51.C	-5.349645	3.770869	0.011118
52.N	-4.563062	2.709603	0.069311
53.O	-0.271495	2.190227	3.140079
54.C	2.808840	4.058960	3.316979
55.N	4.559459	-3.179023	-3.288602
56.N	1.884461	3.026868	3.239118

57.C	3.205654	-0.524812	3.207328
58.H	6.802996	3.202154	-3.238046
59.C	4.620003	3.242755	0.000451
60.H	2.513005	-1.674488	-3.122483
61.O	2.197311	0.234689	3.136133
62.N	3.034260	-1.921138	3.235026
63.N	2.457586	5.354293	3.361142
64.C	1.124562	5.545462	3.323654
65.N	5.557492	-0.123119	0.074566
66.N	5.807507	-1.218620	-3.214844
67.C	4.066544	-2.845419	3.311073
68.C	5.714718	0.127890	-3.211108
69.N	3.733724	-4.149561	3.359913
70.N	5.361973	-2.494131	3.351474
71.C	-3.261791	3.211288	0.067947
72.C	-2.008345	2.549396	0.144895
73.H	-0.909629	-7.720729	3.355478
74.N	-0.484388	-6.798165	3.321867
75.C	0.871759	-6.521969	3.265598
76.N	1.112123	-5.220696	3.234887
77.C	-0.142450	-4.612238	3.267711
78.C	-0.516963	-3.242058	3.214024
79.O	0.242404	-2.233882	3.139067
80.N	-1.913165	-3.070458	3.246352
81.C	-2.837301	-4.102498	3.327116
82.N	-4.141273	-3.769453	3.380183
83.N	-2.486074	-5.397900	3.368295
84.C	-1.153281	-5.589209	3.324121
85.O	-1.793275	1.304765	0.218993
86.N	-0.928167	3.449665	0.134528
87.C	-1.049101	4.833116	0.074882
88.N	0.082739	5.555519	0.086363
89.N	-2.234791	5.460183	0.018860
90.C	-3.283269	4.618220	0.014593
91.C	5.553025	-1.161136	3.312214
92.H	1.617921	-7.305864	3.250138
93.H	-2.228223	-2.077378	3.207539
94.H	-4.486633	-2.792035	3.280684
95.H	-4.805568	-4.534077	3.333717
96.C	0.905654	-4.592447	-3.204008
97.C	0.253038	-3.332482	-3.150112
98.O	0.784439	-2.188043	-3.109168
99.H	6.392710	-3.801515	-0.035275
100.H	-0.048809	-3.040791	0.180381
101.H	-1.073331	-5.175544	0.077503
102.H	-6.431592	3.759690	-0.005929
103.H	0.010795	2.998307	0.181089
104.H	1.034985	5.133180	0.076317
105.H	-0.017565	6.559449	-0.004448
106.H	-5.933388	-5.010562	-0.062418
107.N	-4.993144	-4.626316	-0.027522
108.C	-3.810914	-5.351569	0.008977
109.N	-2.749698	-4.564922	0.066879
110.C	-3.251515	-3.263723	0.067865
111.C	-2.589594	-2.010338	0.145581
112.O	-1.344842	-1.795385	0.218158
113.N	-3.489932	-0.930227	0.138037
114.C	-4.873450	-1.051187	0.079797
115.N	-5.595873	0.080611	0.093718
116.N	-5.500514	-2.236829	0.022724
117.C	-4.658500	-3.285267	0.016161
118.H	-0.021108	-6.601739	-0.009767
119.H	7.269067	1.610686	3.247601
120.H	2.041116	-2.236114	3.197458
121.H	2.755975	-4.494672	3.263090
122.H	4.498269	-4.813766	3.311381
123.N	-1.151222	-3.456310	-3.126591
124.C	-1.840146	-4.659239	-3.189843
125.H	-3.799520	-6.433502	-0.009300

126.H	-3.038613	0.008692	0.185928
127.H	-5.173599	1.032896	0.085361
128.H	-6.599949	-0.019568	0.004399
129.N	-3.184686	-4.605118	-3.269663
130.N	-1.224070	-5.853137	-3.202318
131.C	0.122426	-5.760360	-3.203460
132.H	-0.866135	7.751653	-3.212045
133.N	-1.084751	6.759032	-3.202037
134.C	-2.353495	6.199393	-3.214256
135.N	-2.314825	4.876536	-3.213785
136.C	-0.956848	4.552530	-3.196551
137.C	-0.304062	3.292473	-3.146705
138.O	-0.835388	2.148047	-3.105086
139.H	-7.797163	-0.860662	-3.203657
140.N	-6.804537	-1.079286	-3.195035
141.C	-6.244910	-2.348004	-3.210120
142.N	-4.922060	-2.309306	-3.211261
143.C	-4.598031	-0.951362	-3.192139
144.C	-3.337947	-0.298653	-3.142336
145.O	-2.193449	-0.829989	-3.102505
146.N	-3.461691	1.105652	-3.121838
147.C	-4.664715	1.794439	-3.184479
148.N	-4.610692	3.138801	-3.268244
149.N	-5.858647	1.178390	-3.192927
150.C	-5.765931	-0.168119	-3.190943
151.N	1.100281	3.416210	-3.128799
152.N	-6.790581	0.447769	3.335700
153.C	-0.900971	6.477855	3.276209
154.C	-0.173593	5.720410	-3.198164
155.Na	-0.016272	-0.021794	1.935523
156.K	-0.022662	-0.020935	-1.577996
157.H	3.196509	-6.848886	-3.239445
158.H	-6.854571	-3.242279	-3.216883
159.H	-2.563850	1.633943	-3.111565
160.H	-3.735019	3.692343	-3.190762
161.H	-5.495307	3.629417	-3.196479
162.H	3.623930	5.449622	-3.210165
163.H	1.628571	2.518379	-3.118383
164.H	-1.679525	-2.558514	-3.113161
165.H	-3.675156	-5.489896	-3.199382
166.H	-3.738123	-3.729490	-3.190950
167.H	0.880353	7.676984	3.358935
168.H	4.969533	-5.935076	-0.088895
169.N	4.585440	-4.994901	-0.050584
170.C	5.310844	-3.812793	-0.013635
171.C	1.788956	4.619165	-3.194207
172.N	3.133162	4.565009	-3.280728
173.N	1.172921	5.813085	-3.202842
174.H	-1.647359	7.261607	3.265519
175.N	4.524425	-2.751663	0.048955
176.C	3.223198	-3.253426	0.052677
177.H	3.000450	-0.051014	0.174290
178.H	2.199456	2.033877	3.198688
179.H	4.458040	2.748420	3.264791
180.H	4.777246	4.490685	3.317491
181.C	1.970040	-2.591709	0.135426
182.O	1.755094	-1.347151	0.211132
183.N	0.455368	6.754281	3.326324
184.H	3.686743	3.689377	-3.202929
185.H	3.761592	6.391037	-0.022856
186.N	0.889927	-3.492087	0.129092
187.C	1.010685	-4.875452	0.067251
188.H	-7.713164	0.872889	3.369964
189.N	-1.141204	5.176588	3.244803
190.C	0.113630	4.568367	3.270823
191.C	0.488111	3.198361	3.213316
192.N	-0.121042	-5.597905	0.082551
193.N	2.196189	-5.502375	0.005463
194.N	5.461999	2.194322	0.004343

Table S16 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–K^+–G_4–K^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–K^+–G_4–K^+–G_4 (Bond Energy: -29819.07 kcal/mol)			
1.C	-6.571466	-0.895351	3.148447
2.N	-5.274449	-1.149092	3.224934
3.C	-4.660089	0.103110	3.250355
4.C	-3.287489	0.461730	3.312805
5.O	-2.288065	-0.309302	3.355347
6.N	-3.098584	1.858441	3.318460
7.C	-4.122311	2.794608	3.302383
8.N	-3.777769	4.098941	3.389338
9.N	-5.419314	2.458174	3.238094
10.C	-5.624862	1.125230	3.201495
11.C	3.835073	-4.225066	0.010262
12.H	0.323934	-7.811093	-3.243936
13.N	0.606270	-6.834633	-3.242379
14.H	5.283791	5.703322	-0.007494
15.N	4.396516	5.207507	-0.007483
16.C	3.134880	5.784596	-0.041806
17.C	1.908372	-6.358222	-3.218776
18.H	-7.361956	-1.633438	3.103253
19.H	-2.106657	2.175775	3.353668
20.H	-2.801740	4.440733	3.285379
21.H	-4.525804	4.763663	3.220993
22.N	1.955368	-5.035185	-3.230210
23.H	7.811550	0.323926	-3.240461
24.N	6.835071	0.606216	-3.239548
25.C	6.358542	1.908271	-3.216248
26.N	2.173210	4.877572	-0.039980
27.C	2.321909	2.324396	0.022959
28.N	5.035495	1.955152	-3.228567
29.C	4.624980	0.621726	-3.255819
30.C	3.324837	0.053017	-3.241837
31.O	2.216922	0.659385	-3.226065
32.N	3.356520	-1.356611	-3.236785
33.H	-5.703000	5.283229	-0.007676
34.H	3.464012	-3.956315	-3.237021
35.N	-5.207128	4.395987	-0.007418
36.H	5.226805	-4.007016	-3.238245
37.H	5.250194	-0.397730	-0.019507
38.N	3.342780	1.355354	0.034800
39.N	4.098175	3.777152	3.388655
40.H	6.540898	0.815625	-0.013168
41.C	4.703857	1.638208	0.021858
42.C	2.829875	3.646858	-0.006116
43.O	1.109276	1.962190	0.043797
44.H	7.756178	-0.897808	3.090880
45.N	6.836801	-0.465742	3.127451
46.C	6.571466	0.895351	3.148447
47.N	5.274449	1.149092	3.224934
48.C	4.513821	-2.121292	-3.272842
49.C	4.660089	-0.103110	3.250355
50.H	-2.761220	7.024094	-3.193299
51.C	-5.784166	3.134305	-0.040355
52.N	-4.877097	2.172672	-0.037877
53.O	-0.310286	2.288138	3.355465
54.C	2.793934	4.121897	3.301368
55.N	4.374714	-3.462102	-3.308671
56.N	1.857527	3.098368	3.318001
57.C	3.287489	-0.461730	3.312805
58.H	7.024318	2.761175	-3.190232
59.C	4.225526	3.835459	0.010367
60.H	2.426203	-1.824670	-3.234463
61.O	2.288065	0.309302	3.355347
62.N	3.098584	-1.858441	3.318460

63.N	2.457700	5.418893	3.236280
64.C	1.124795	5.624656	3.199492
65.N	5.551717	0.598222	-0.015067
66.N	5.744601	-1.584205	-3.287359
67.C	4.122311	-2.794608	3.302383
68.C	5.739593	-0.235804	-3.264601
69.N	3.777769	-4.098941	3.389338
70.N	5.419314	-2.458174	3.238094
71.C	-3.646394	2.829415	-0.004962
72.C	-2.323893	2.321507	0.024197
73.H	-0.897790	-7.755996	3.088133
74.N	-0.465545	-6.836699	3.124883
75.C	0.895592	-6.571648	3.146088
76.N	1.149605	-5.274708	3.223161
77.C	-0.102481	-4.660097	3.248812
78.C	-0.460871	-3.287485	3.312219
79.O	0.310286	-2.288138	3.355465
80.N	-1.857527	-3.098368	3.318001
81.C	-2.793934	-4.121897	3.301368
82.N	-4.098175	-3.777152	3.388655
83.N	-2.457700	-5.418893	3.236280
84.C	-1.124795	-5.624656	3.199492
85.O	-1.961841	1.108806	0.046394
86.N	-1.354894	3.342419	0.034410
87.C	-1.637854	4.703483	0.020570
88.N	-0.597937	5.551407	-0.017178
89.N	-2.892147	5.185309	0.033435
90.C	-3.835073	4.225066	0.010262
91.C	5.624862	-1.125230	3.201495
92.H	1.633523	-7.362269	3.100518
93.H	-2.174542	-2.106494	3.353683
94.H	-4.439900	-2.800993	3.285666
95.H	-4.763055	-4.524952	3.219930
96.C	0.621958	-4.624539	-3.257167
97.C	0.053382	-3.324350	-3.242035
98.O	0.659969	-2.216583	-3.225261
99.H	6.856976	-2.995938	-0.063409
100.H	0.367154	-3.010855	0.040911
101.H	-0.398062	-5.250076	-0.021849
102.H	-6.856976	2.995938	-0.063409
103.H	-0.367154	3.010855	0.040911
104.H	0.398062	5.250076	-0.021849
105.H	-0.815464	6.540564	-0.016446
106.H	-5.283791	-5.703322	-0.007494
107.N	-4.396516	-5.207507	-0.007483
108.C	-3.134880	-5.784596	-0.041806
109.N	-2.173210	-4.877572	-0.039980
110.C	-2.829875	-3.646858	-0.006116
111.C	-2.321909	-2.324396	0.022959
112.O	-1.109276	-1.962190	0.043797
113.N	-3.342780	-1.355354	0.034800
114.C	-4.703857	-1.638208	0.021858
115.N	-5.551717	-0.598222	-0.015067
116.N	-5.185715	-2.892500	0.034708
117.C	-4.225526	-3.835459	0.010367
118.H	0.815464	-6.540564	-0.016446
119.H	7.361956	1.633438	3.103253
120.H	2.106657	-2.175775	3.353668
121.H	2.801740	-4.440733	3.285379
122.H	4.525804	-4.763663	3.220993
123.N	-1.356281	-3.355848	-3.237104
124.C	-2.121028	-4.513100	-3.274004
125.H	-2.996590	-6.857407	-0.065260
126.H	-3.010940	-0.367767	0.041851
127.H	-5.250194	0.397730	-0.019507
128.H	-6.540898	-0.815625	-0.013168
129.N	-3.461838	-4.373935	-3.309912
130.N	-1.584049	-5.743917	-3.289350
131.C	-0.235648	-5.739063	-3.266677

132.H	-0.323934	7.811093	-3.243936
133.N	-0.606270	6.834633	-3.242379
134.C	-1.908372	6.358222	-3.218776
135.N	-1.955368	5.035185	-3.230210
136.C	-0.621958	4.624539	-3.257167
137.C	-0.053382	3.324350	-3.242035
138.O	-0.659969	2.216583	-3.225261
139.H	-7.811550	-0.323926	-3.240461
140.N	-6.835071	-0.606216	-3.239548
141.C	-6.358542	-1.908271	-3.216248
142.N	-5.035495	-1.955152	-3.228567
143.C	-4.624980	-0.621726	-3.255819
144.C	-3.324837	-0.053017	-3.241837
145.O	-2.216922	-0.659385	-3.226065
146.N	-3.356520	1.356611	-3.236785
147.C	-4.513821	2.121292	-3.272842
148.N	-4.374714	3.462102	-3.308671
149.N	-5.744601	1.584205	-3.287359
150.C	-5.739593	0.235804	-3.264601
151.N	1.356281	3.355848	-3.237104
152.N	-6.836801	0.465742	3.127451
153.C	-0.895592	6.571648	3.146088
154.C	0.235648	5.739063	-3.266677
155.K	0.000000	0.000000	1.827215
156.K	0.000000	0.000000	-1.732388
157.H	2.761220	-7.024094	-3.193299
158.H	-7.024318	-2.761175	-3.190232
159.H	-2.426203	1.824670	-3.234463
160.H	-3.464012	3.956315	-3.237021
161.H	-5.226805	4.007016	-3.238245
162.H	4.006705	5.226107	-3.239979
163.H	1.824437	2.425522	-3.234651
164.H	-1.824437	-2.425522	-3.234651
165.H	-4.006705	-5.226107	-3.239979
166.H	-3.956100	-3.463362	-3.237011
167.H	0.897790	7.755996	3.088133
168.H	5.703000	-5.283229	-0.007676
169.N	5.207128	-4.395987	-0.007418
170.C	5.784166	-3.134305	-0.040355
171.C	2.121028	4.513100	-3.274004
172.N	3.461838	4.373935	-3.309912
173.N	1.584049	5.743917	-3.289350
174.H	-1.633523	7.362269	3.100518
175.N	4.877097	-2.172672	-0.037877
176.C	3.646394	-2.829415	-0.004962
177.H	3.010940	0.367767	0.041851
178.H	2.174542	2.106494	3.353683
179.H	4.439900	2.800993	3.285666
180.H	4.763055	4.524952	3.219930
181.C	2.323893	-2.321507	0.024197
182.O	1.961841	-1.108806	0.046394
183.N	0.465545	6.836699	3.124883
184.H	3.956100	3.463362	-3.237011
185.H	2.996590	6.857407	-0.065260
186.N	1.354894	-3.342419	0.034410
187.C	1.637854	-4.703483	0.020570
188.H	-7.756178	0.897808	3.090880
189.N	-1.149605	5.274708	3.223161
190.C	0.102481	4.660097	3.248812
191.C	0.460871	3.287485	3.312219
192.N	0.597937	-5.551407	-0.017178
193.N	2.892147	-5.185309	0.033435
194.N	5.185715	2.892500	0.034708

Table S17 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **G_4–K^+–G_4–Rb^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–K^+–G_4–Rb^+–G_4 (Bond Energy: -29810.86 kcal/mol)

1.C	-6.595996	-0.708893	3.098277
2.N	-5.313688	-0.997358	3.257419
3.C	-4.666259	0.238494	3.286186
4.C	-3.291160	0.559614	3.431683
5.O	-2.320607	-0.237386	3.566308
6.N	-3.059319	1.951246	3.402110
7.C	-4.052048	2.915511	3.296102
8.N	-3.674228	4.212604	3.364675
9.N	-5.352089	2.613173	3.166695
10.C	-5.595368	1.285738	3.153898
11.C	3.933950	-4.151826	0.009829
12.H	0.385400	-7.801378	-3.215515
13.N	0.662642	-6.823524	-3.228063
14.H	5.223982	5.815804	-0.011245
15.N	4.343155	5.308691	-0.023414
16.C	3.074699	5.870366	-0.072069
17.C	1.961973	-6.339901	-3.205511
18.H	-7.404372	-1.425039	3.025047
19.H	-2.065457	2.246793	3.491970
20.H	-2.687356	4.526718	3.289830
21.H	-4.391703	4.889940	3.126883
22.N	2.002218	-5.016801	-3.236187
23.H	7.830343	0.375096	-3.240337
24.N	6.852440	0.652262	-3.250620
25.C	6.368839	1.951644	-3.230610
26.N	2.123981	4.952115	-0.088983
27.C	2.304682	2.401863	-0.053834
28.N	5.045651	1.991758	-3.257364
29.C	4.642661	0.656118	-3.290460
30.C	3.345413	0.080507	-3.296179
31.O	2.234386	0.681214	-3.298412
32.N	3.384539	-1.328997	-3.288943
33.H	-5.778324	5.224896	-0.014430
34.H	3.506552	-3.927400	-3.263948
35.N	-5.271200	4.344049	-0.024601
36.H	5.268367	-3.968815	-3.252913
37.H	5.269816	-0.288206	-0.053604
38.N	3.336391	1.443609	-0.030230
39.N	4.199257	3.721122	3.370950
40.H	6.540811	0.941291	-0.020609
41.C	4.694305	1.742400	-0.015783
42.C	2.796253	3.730020	-0.051121
43.O	1.096445	2.024882	-0.068003
44.H	7.755581	-1.057240	2.935003
45.N	6.852506	-0.600486	3.030425
46.C	6.629044	0.767188	3.093612
47.N	5.346737	1.056752	3.250669
48.C	4.546230	-2.087425	-3.309772
49.C	4.699298	-0.178893	3.287718
50.H	-2.778892	7.019618	-3.213405
51.C	-5.832925	3.075387	-0.066971
52.N	-4.914659	2.124662	-0.082716
53.O	-0.251530	2.367518	3.553977
54.C	2.902455	4.098628	3.294875
55.N	4.414487	-3.429703	-3.345139
56.N	1.937795	3.106027	3.398330
57.C	3.324234	-0.498996	3.435564
58.H	7.029744	2.808042	-3.195854
59.C	4.189273	3.934869	-0.014417
60.H	2.456841	-1.802133	-3.294333
61.O	2.353691	0.298899	3.564809
62.N	3.092359	-1.890823	3.415686
63.N	2.600619	5.398322	3.161032
64.C	1.273236	5.641451	3.141394
65.N	5.554563	0.712189	-0.047451
66.N	5.773957	-1.543939	-3.312302
67.C	4.085112	-2.855800	3.316247

68.C	5.761785	-0.195535	-3.287978
69.N	3.707311	-4.152391	3.393609
70.N	5.385119	-2.554325	3.184609
71.C	-3.692514	2.797120	-0.050688
72.C	-2.364346	2.305618	-0.055123
73.H	-1.069335	-7.710157	2.954278
74.N	-0.612921	-6.806848	3.049096
75.C	0.754523	-6.583202	3.116400
76.N	1.043525	-5.300522	3.271473
77.C	-0.192244	-4.653030	3.302823
78.C	-0.512891	-3.277605	3.446189
79.O	0.284554	-2.306727	3.575830
80.N	-1.904625	-3.045798	3.420724
81.C	-2.869230	-4.038797	3.320218
82.N	-4.166104	-3.660820	3.391978
83.N	-2.567291	-5.339143	3.193010
84.C	-1.239917	-5.582461	3.176327
85.O	-1.987367	1.097321	-0.066087
86.N	-1.406091	3.337430	-0.037616
87.C	-1.704928	4.695374	-0.027484
88.N	-0.674852	5.555556	-0.064946
89.N	-2.964864	5.161625	0.005350
90.C	-3.897351	4.190267	-0.018660
91.C	5.628408	-1.227018	3.162631
92.H	1.470418	-7.391763	3.042731
93.H	-2.199878	-2.051717	3.509163
94.H	-4.480457	-2.674149	3.315386
95.H	-4.844129	-4.378885	3.157955
96.C	0.666694	-4.613872	-3.274631
97.C	0.091152	-3.316635	-3.286192
98.O	0.691884	-2.205632	-3.289995
99.H	6.940872	-2.886707	-0.060526
100.H	0.450111	-2.983777	-0.038496
101.H	-0.288977	-5.232510	-0.039081
102.H	-6.904197	2.924652	-0.082606
103.H	-0.413415	3.021968	-0.055785
104.H	0.325523	5.270776	-0.072239
105.H	-0.903931	6.541881	-0.040788
106.H	-5.187624	-5.777225	0.024355
107.N	-4.306781	-5.270235	0.008587
108.C	-3.038340	-5.832252	-0.036408
109.N	-2.087598	-4.914167	-0.059451
110.C	-2.759822	-3.691844	-0.029520
111.C	-2.268232	-2.363780	-0.041076
112.O	-1.059947	-1.986966	-0.057887
113.N	-3.299864	-1.405330	-0.023564
114.C	-4.657798	-1.703963	-0.006728
115.N	-5.518004	-0.673921	-0.044478
116.N	-5.124020	-2.963708	0.032793
117.C	-4.152851	-3.896391	0.008596
118.H	0.940330	-6.503417	0.002523
119.H	7.437444	1.482801	3.015627
120.H	2.098642	-2.185761	3.508937
121.H	2.720456	-4.467072	3.321013
122.H	4.424819	-4.831336	3.160563
123.N	-1.318380	-3.355721	-3.283248
124.C	-2.076771	-4.517449	-3.302805
125.H	-2.887773	-6.903599	-0.048384
126.H	-2.984394	-0.412759	-0.046617
127.H	-5.233165	0.326405	-0.057020
128.H	-6.504236	-0.902772	-0.014987
129.N	-3.418934	-4.385794	-3.342869
130.N	-1.533315	-5.745183	-3.299710
131.C	-0.185000	-5.732962	-3.271323
132.H	-0.346009	7.819882	-3.266628
133.N	-0.623264	6.841969	-3.272771
134.C	-1.922628	6.358532	-3.247985
135.N	-1.962906	5.035267	-3.270154
136.C	-0.627366	4.632070	-3.305046

137.C	-0.051852	3.334784	-3.308024
138.O	-0.652631	2.223780	-3.305511
139.H	-7.791368	-0.356060	-3.240643
140.N	-6.813502	-0.633422	-3.248830
141.C	-6.330067	-1.932709	-3.220142
142.N	-5.006877	-1.973173	-3.246265
143.C	-4.603711	-0.637815	-3.287938
144.C	-3.306405	-0.062410	-3.297406
145.O	-2.195440	-0.663243	-3.295884
146.N	-3.345329	1.347124	-3.299361
147.C	-4.506936	2.105546	-3.325127
148.N	-4.374984	3.447538	-3.369104
149.N	-5.734717	1.562186	-3.324354
150.C	-5.722724	0.213979	-3.291272
151.N	1.357679	3.373798	-3.304206
152.N	-6.819452	0.658323	3.025764
153.C	-0.721198	6.641799	3.074547
154.C	0.224367	5.751131	-3.308359
155.Rb	0.017340	0.022802	1.867447
156.K	0.018427	0.014414	-1.807405
157.H	2.818230	-7.000728	-3.166107
158.H	-6.991100	-2.788770	-3.179984
159.H	-2.417599	1.820145	-3.307762
160.H	-3.466996	3.945646	-3.290972
161.H	-5.228793	3.987360	-3.280461
162.H	3.997717	5.257546	-3.280648
163.H	1.830734	2.446044	-3.307610
164.H	-1.791518	-2.428063	-3.293211
165.H	-3.958334	-5.239367	-3.249467
166.H	-3.916883	-3.477637	-3.265853
167.H	1.102799	7.768089	2.909267
168.H	5.814995	-5.186394	0.022312
169.N	5.307812	-4.305663	0.005836
170.C	5.869584	-3.037317	-0.044650
171.C	2.116137	4.535369	-3.330550
172.N	3.458303	4.403414	-3.368650
173.N	1.572704	5.763118	-3.335907
174.H	-1.437046	7.449978	2.996410
175.N	4.951369	-2.086714	-0.067640
176.C	3.729200	-2.758930	-0.031873
177.H	3.020976	0.450916	-0.047455
178.H	2.232996	2.112524	3.493184
179.H	4.513749	2.734141	3.299103
180.H	4.877631	4.438175	3.134812
181.C	2.401070	-2.267428	-0.040641
182.O	2.024090	-1.059247	-0.059769
183.N	0.646316	6.865207	3.007785
184.H	3.956183	3.495688	-3.286199
185.H	2.924090	6.941598	-0.091137
186.N	1.442760	-3.299085	-0.017102
187.C	1.741515	-4.656930	0.003021
188.H	-7.722500	1.114430	2.927034
189.N	-1.010302	5.359804	3.235051
190.C	0.225464	4.712545	3.270755
191.C	0.546006	3.337812	3.420791
192.N	0.711382	-5.517271	-0.028982
193.N	3.001402	-5.122977	0.040081
194.N	5.160496	3.002388	0.015677

Table S18 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K$^+$–[ ]** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–K$^+$–[ ] (Bond Energy: -55747.80 kcal/mol)			
1.C	6.518223	-1.331888	2.810541
2.N	5.406310	-0.711288	3.159600
3.C	4.405917	-1.686029	3.129771
4.C	3.002805	-1.584329	3.353708

5.O	2.338117	-0.553171	3.631139
6.N	2.354512	-2.835161	3.223671
7.C	2.997884	-4.031675	2.947961
8.N	2.261440	-5.165001	2.958287
9.N	4.314881	-4.116344	2.700982
10.C	4.948184	-2.932422	2.786527
11.H	10.358315	-2.356502	3.893630
12.H	11.460247	-2.422907	2.468285
13.H	10.317921	-4.548467	2.564795
14.H	10.100610	-3.073925	0.219557
15.H	7.996217	-2.030870	0.756100
16.H	7.426073	-3.406207	-0.174465
17.H	6.739268	-4.591405	1.884797
18.H	7.510316	-0.902884	2.720856
19.H	1.320358	-2.817280	3.355414
20.H	1.223960	-5.178159	3.001661
21.H	2.721101	-5.987983	2.582355
22.P	9.110004	-5.450308	-1.328876
23.O	10.224047	-6.732149	-1.707795
24.O	9.040923	-4.132515	-2.255946
25.O	7.625213	-6.355451	-1.311859
26.C	7.644096	-7.663201	-0.493767
27.C	-2.789066	-1.707260	-0.085577
28.C	6.248073	-8.272354	-0.503290
29.O	5.280382	-7.354995	0.209115
30.C	5.618237	-8.521240	-1.890085
31.O	4.644880	-9.687431	-1.593274
32.C	4.843391	-7.234584	-2.172236
33.C	4.240132	-6.906130	-0.790140
34.H	-2.737066	4.599799	-3.360155
35.N	3.955341	-5.513776	-0.572418
36.H	-4.473880	4.932501	-3.371561
37.H	-4.961946	1.651673	-0.117037
38.N	-3.541243	-0.515395	0.007198
39.N	-5.056756	-2.327731	3.091978
40.H	-6.491139	0.789793	-0.336367
41.C	-4.925922	-0.437869	-0.072642
42.H	-6.548613	-5.508178	-2.372259
43.O	-1.531927	-1.661198	-0.053324
44.H	-7.422221	-4.011743	-2.802640
45.H	-9.826138	0.747706	0.017889
46.H	-11.201323	0.127259	-2.299568
47.H	-9.264009	-0.132629	-3.756090
48.H	-9.703832	1.569441	-4.067486
49.H	-7.867866	2.388792	-2.705599
50.H	1.506624	-7.255024	-3.328420
51.C	4.840069	-4.437686	-0.607237
52.N	4.220785	-3.286175	-0.434821
53.O	-0.423241	-2.414841	3.593798
54.C	-3.924308	-3.062483	3.023855
55.C	-2.302127	-10.469990	2.629484
56.N	-2.718918	-2.424733	3.272529
57.H	-12.407282	-3.495567	-1.905035
58.H	-7.367527	-1.422087	-3.117901
59.C	-5.007091	-2.667232	-0.266495
60.H	-2.062647	2.314449	-3.398261
61.H	3.524585	-12.335189	-2.214025
62.H	11.186508	-6.446077	-1.775970
63.N	-4.017194	-4.373110	2.747665
64.C	-2.830683	-5.006796	2.774339
65.N	-5.505551	0.771503	-0.051237
66.O	1.171556	9.625163	2.544853
67.C	2.343236	10.296669	3.202580
68.C	3.623976	9.614235	2.724793
69.O	3.789350	8.256424	3.382357
70.C	3.631741	9.337676	1.212418

71.O	5.120721	9.437362	0.814356
72.C	3.113575	7.909257	1.074006
73.C	3.599553	7.174705	2.344266
74.N	2.639502	6.200899	2.829356
75.C	1.274453	6.410474	3.050928
76.N	0.645866	5.288800	3.351018
77.C	1.620906	4.288938	3.312130
78.C	1.514458	2.880243	3.493915
79.O	0.477777	2.208744	3.732106
80.N	2.767469	2.234897	3.370612
81.C	3.969839	2.885266	3.140124
82.N	5.102271	2.147585	3.151105
83.N	4.060394	4.209325	2.936633
84.C	2.874876	4.840631	3.014586
85.H	2.268179	10.204000	4.293865
86.H	2.369030	11.356711	2.911452
87.H	4.493348	10.213143	3.020815
88.H	3.078708	10.078803	0.632277
89.H	2.026390	7.957188	1.063947
90.H	3.427443	7.421208	0.151405
91.H	4.556242	6.659113	2.214563
92.H	0.847765	7.405228	2.982347
93.H	2.746194	1.196883	3.467270
94.H	5.114101	1.109239	3.163335
95.H	5.932920	2.617247	2.805747
96.P	5.496072	9.156300	-0.890409
97.O	6.789796	10.280403	-1.188875
98.O	4.202230	9.127696	-1.852944
99.O	6.398012	7.669049	-0.909126
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101.C	8.294252	6.258306	-0.107413
102.O	7.360295	5.267752	0.549417
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104.O	9.735093	4.695185	-1.221342
105.C	7.294466	4.913909	-1.847798
106.C	6.933559	4.263417	-0.495521
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117.C	5.009214	2.695890	-0.174241
118.H	7.410639	7.902056	0.968044
119.H	8.372711	8.395284	-0.484515
120.H	9.220305	6.281590	0.482176
121.H	8.911637	6.402989	-2.254072
122.H	6.535734	5.651928	-2.132421
123.H	7.405943	4.182668	-2.653626
124.H	7.479868	3.333560	-0.329563
125.H	4.627557	5.918983	-0.484678
126.H	2.973900	-0.342240	0.009280
127.H	4.962048	-1.624725	-0.255503
128.H	6.489943	-0.753211	-0.444212
129.P	10.129584	3.433211	-2.392619
130.O	11.660219	2.899183	-1.766577
131.O	9.944220	3.822332	-3.946131
132.O	9.152724	2.048908	-2.013750
133.C	9.347579	1.244023	-0.720521
134.C	9.469244	-0.246145	-1.035598
135.O	8.123097	-0.852811	-1.332598
136.C	10.330707	-0.636533	-2.257348

137.O	10.940243	-1.993212	-2.047494
138.C	9.333661	-0.637335	-3.438897
139.C	8.000415	-1.129877	-2.822885
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143.C	4.618546	-0.067144	-3.484241
144.C	3.238735	-0.406942	-3.484716
145.O	2.248813	0.373911	-3.433256
146.N	3.032304	-1.801930	-3.516836
147.C	4.043616	-2.747514	-3.558055
148.N	3.688368	-4.040936	-3.688021
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150.C	5.563190	-1.101851	-3.431446
151.H	8.445750	1.427819	-0.130272
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153.H	9.828048	-0.733595	-0.120163
154.H	11.178651	0.037953	-2.405046
155.H	9.227437	0.380453	-3.827670
156.H	9.671232	-1.296812	-4.247824
157.H	7.849362	-2.207362	-2.925941
158.H	7.337691	1.620256	-3.104058
159.H	2.033028	-2.101523	-3.531124
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161.H	4.445232	-4.714197	-3.685734
162.H	-4.841633	-4.350525	-3.636469
163.H	-2.223748	-1.942106	-3.511131
164.P	-10.149447	-3.288909	-2.493137
165.O	-11.683304	-2.800400	-1.837278
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167.O	-9.184841	-1.913163	-2.053140
168.H	-2.213686	-10.447996	3.723546
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170.H	-4.454326	-10.370358	2.482952
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172.H	-3.417820	-7.411052	-0.225852
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175.C	-9.364637	-1.190745	-0.710152
176.H	-0.299560	-10.202266	2.314054
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185.O	-6.406468	-7.588974	-1.268910
186.C	-7.686936	-7.624218	-0.409568
187.C	-8.293892	-6.227826	-0.371574
188.O	-7.353877	-5.276415	0.333213
189.C	-8.583015	-5.568901	-1.737017
190.O	-9.739704	-4.602796	-1.385881
191.C	-7.305071	-4.787709	-2.040610
192.O	-5.109376	-9.456628	0.336451
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195.C	-9.479267	0.316911	-0.929883
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200.C	-4.461479	-4.817955	-0.568822
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208.C	-4.650022	0.281929	-3.431741
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212.C	-3.616893	-2.853691	-0.234127
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214.O	-3.738441	-8.440766	2.953724
215.O	-10.951609	2.130537	-1.814330
216.C	-3.614624	-9.387888	0.719771
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218.O	9.718275	-1.215034	2.195347
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224.C	9.379291	-3.640460	0.811648
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226.H	-8.461004	-1.416142	-0.137397
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228.C	2.867934	-3.603773	-0.293087
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254.C	-0.720600	-10.267604	-2.477961
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274.C	-3.563292	-7.298596	1.979908
275.H	-9.215522	-6.283611	0.222719
276.O	-8.132443	0.934705	-1.200038
277.H	-0.051699	-11.111254	-2.668901
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279.N	-4.168327	-3.593698	-3.642202
280.N	-2.550006	-5.255746	-3.528079
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282.O	-1.136819	-9.759183	2.002504
283.H	-7.478860	-3.295802	-0.433766
284.C	7.947444	-3.117914	0.738297
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287.H	-2.312988	-7.771974	-3.034058
288.H	-8.926278	-6.251270	-2.518422
289.C	7.258675	-3.637621	2.020930
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293.O	-9.680395	1.096579	2.353288
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296.O	-8.324967	3.676076	3.317267
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314.H	-10.268827	4.402595	2.930776
315.H	-10.078602	3.076948	0.496677
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317.H	-7.407460	3.422607	0.097714
318.H	-6.697098	4.478039	2.217460
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320.H	-1.271205	2.617680	3.537141
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322.H	-2.673571	5.826271	2.946188
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325.O	-9.051614	4.276682	-1.917469
326.O	-7.629905	6.449180	-0.873178
327.C	-7.636988	7.709573	0.015887
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329.O	-5.266823	7.356720	0.673990
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331.O	-4.647605	9.787125	-1.006537
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346.H	-8.366719	8.409182	-0.402468
347.H	-6.274244	9.220936	0.642666
348.H	-6.331379	8.999724	-2.104843
349.H	-5.587098	6.620142	-2.041718
350.H	-4.103602	7.502568	-2.498226
351.H	-3.311916	7.499066	-0.153143
352.H	-5.897553	4.658427	-0.460233
353.H	0.350470	2.979426	0.110322
354.H	1.639706	4.973410	-0.059627
355.H	0.773015	6.508034	-0.214172
356.P	-3.363099	10.220024	-2.139444
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358.O	-3.720159	10.083370	-3.705605
359.O	-1.986525	9.231265	-1.762286
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362.O	0.895168	8.170230	-1.039015
363.C	0.704579	10.408178	-1.894015
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366.C	1.210559	8.097098	-2.524752
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370.C	0.161897	4.741537	-3.327826
371.C	0.501064	3.362123	-3.369470
372.O	-0.280933	2.371929	-3.369921
373.N	1.896351	3.155212	-3.377539
374.C	2.842986	4.166284	-3.361510
375.N	4.138800	3.814403	-3.476498
376.N	2.521586	5.466000	-3.249657
377.C	1.195450	5.682471	-3.218694
378.H	-1.416631	8.455162	0.110497
379.H	-1.583795	10.261079	0.090090
380.H	0.745520	9.832495	0.226926
381.H	0.034003	11.261030	-2.030818
382.H	-0.271826	9.359912	-3.526344
383.H	1.416167	9.814546	-3.887740
384.H	2.290215	7.947361	-2.605453
385.H	-1.532588	7.448084	-2.892280
386.H	2.195249	2.156472	-3.418016
387.H	4.479806	2.832506	-3.445143
388.H	10.235939	-2.709459	-2.152287
389.H	-10.247073	2.850651	-1.884822
390.H	-2.788599	-10.176690	-2.295057
391.H	-1.447870	-9.561819	-4.428903
392.H	2.774542	10.309218	-1.740803
393.H	-11.199778	6.541675	-1.275398
394.H	-3.518726	12.472834	-1.516011
395.H	6.504738	11.243504	-1.250288
396.H	-10.113373	0.252712	2.661192
397.H	-6.509907	-11.143421	-1.784272
398.H	12.398368	3.579682	-1.827896
399.H	0.337306	10.045437	2.893897
400.H	10.152129	-0.390338	2.550472

401.K	-0.007502	0.057064	-1.725546

Table S19 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K^+–Li^+** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–K^+–Li^+ (Bond Energy: -55762.05 kcal/mol)			
1.C	6.367370	-1.284249	2.780872
2.N	5.225848	-0.682547	3.057380
3.C	4.247273	-1.679209	3.023839
4.C	2.829916	-1.619074	3.141061
5.O	2.103084	-0.588850	3.287260
6.N	2.236884	-2.889446	3.060405
7.C	2.930928	-4.080192	2.885347
8.N	2.231110	-5.228615	2.933991
9.N	4.258016	-4.128132	2.695562
10.C	4.844607	-2.923876	2.757898
11.H	10.262011	-2.236427	3.937154
12.H	11.359015	-2.304607	2.508184
13.H	10.244832	-4.450763	2.657454
14.H	10.032134	-3.035764	0.276470
15.H	7.918531	-1.993742	0.787884
16.H	7.365174	-3.386215	-0.130436
17.H	6.685370	-4.556980	1.941936
18.H	7.349774	-0.829080	2.716649
19.H	1.198209	-2.876192	3.130661
20.H	1.188902	-5.231290	2.941257
21.H	2.724110	-6.061614	2.629597
22.P	9.096355	-5.442127	-1.237256
23.O	10.232451	-6.718711	-1.563501
24.O	9.038678	-4.138628	-2.185038
25.O	7.619169	-6.359815	-1.251892
26.C	7.627730	-7.673487	-0.443544
27.C	-2.788417	-1.708250	-0.115598
28.C	6.231632	-8.283856	-0.473392
29.O	5.252796	-7.366458	0.223526
30.C	5.619582	-8.536895	-1.867640
31.O	4.636815	-9.697943	-1.577713
32.C	4.852973	-7.249131	-2.165379
33.C	4.230436	-6.915625	-0.793127
34.H	-2.733836	4.604349	-3.374835
35.N	3.947399	-5.522059	-0.583834
36.H	-4.470529	4.939998	-3.387738
37.H	-4.948510	1.662312	-0.170379
38.N	-3.535685	-0.512631	-0.031834
39.N	-5.121263	-2.292887	3.062963
40.H	-6.480888	0.802461	-0.396172
41.C	-4.919161	-0.429357	-0.121956
42.H	-6.566388	-5.526608	-2.354783
43.O	-1.532521	-1.667173	-0.076340
44.H	-7.437993	-4.035012	-2.805488
45.H	-9.798272	0.750491	0.015752
46.H	-11.195822	0.124410	-2.286859
47.H	-9.273250	-0.130113	-3.763783
48.H	-9.723313	1.569914	-4.071771
49.H	-7.873568	2.398173	-2.733229
50.H	1.494883	-7.259878	-3.351595
51.C	4.836452	-4.449964	-0.614108
52.N	4.219821	-3.295783	-0.448974
53.O	-0.471431	-2.168378	3.247775
54.C	-3.975036	-2.990707	2.958030
55.C	-2.197806	-10.368478	2.682509
56.N	-2.778804	-2.299444	3.102793
57.H	-12.410451	-3.459302	-1.880162
58.H	-7.373701	-1.413009	-3.154572
59.C	-5.011094	-2.659823	-0.292926
60.H	-2.063455	2.317412	-3.403862
61.H	3.495730	-12.335843	-2.190164
62.H	11.194822	-6.426540	-1.599508

63.N	-4.029749	-4.313827	2.744257
64.C	-2.823906	-4.900509	2.749894
65.N	-5.492917	0.781721	-0.118612
66.O	1.099430	9.504595	2.574452
67.C	2.251202	10.194616	3.248382
68.C	3.548306	9.530591	2.789408
69.O	3.708294	8.166505	3.436930
70.C	3.589285	9.269193	1.274530
71.O	5.085454	9.373506	0.904546
72.C	3.078508	7.841041	1.113282
73.C	3.554908	7.098118	2.382244
74.N	2.603902	6.097619	2.834766
75.C	1.228295	6.262598	3.006646
76.N	0.618966	5.113656	3.230933
77.C	1.615732	4.135309	3.192372
78.C	1.552200	2.715029	3.263875
79.O	0.518243	1.985104	3.359867
80.N	2.824128	2.123496	3.198588
81.C	4.019372	2.821411	3.079046
82.N	5.166026	2.119351	3.138624
83.N	4.072721	4.153665	2.931607
84.C	2.867248	4.739209	2.978849
85.H	2.162077	10.100017	4.338415
86.H	2.265274	11.255149	2.958221
87.H	4.406221	10.133058	3.110422
88.H	3.046182	10.014790	0.690912
89.H	1.991367	7.885757	1.092805
90.H	3.405427	7.364662	0.189539
91.H	4.521773	6.599896	2.261209
92.H	0.775545	7.247179	2.962678
93.H	2.809141	1.083065	3.237567
94.H	5.168579	1.077428	3.108203
95.H	6.006747	2.620907	2.871593
96.P	5.485387	9.130802	-0.802027
97.O	6.770512	10.273329	-1.065506
98.O	4.202823	9.108844	-1.779657
99.O	6.400049	7.652509	-0.842364
100.C	7.697144	7.632337	-0.008012
101.C	8.307251	6.237372	-0.074897
102.O	7.375663	5.235488	0.567928
103.C	8.587977	5.675488	-1.485127
104.O	9.744491	4.683866	-1.208259
105.C	7.306560	4.920702	-1.835810
106.C	6.943597	4.251006	-0.493606
107.N	5.545448	3.964020	-0.323422
108.C	4.474735	4.854885	-0.351889
109.N	3.316529	4.235016	-0.233466
110.C	3.624635	2.876130	-0.136366
111.C	2.792131	1.726373	-0.049130
112.O	1.536573	1.683211	-0.003140
113.N	3.540140	0.528283	-0.033384
114.C	4.923281	0.450866	-0.135459
115.N	5.497683	-0.758572	-0.197393
116.N	5.708348	1.543094	-0.173288
117.C	5.013557	2.687250	-0.191911
118.H	7.429656	7.866515	1.027595
119.H	8.376234	8.380009	-0.428205
120.H	9.233440	6.253911	0.514618
121.H	8.930068	6.409713	-2.218574
122.H	6.549515	5.664161	-2.110605
123.H	7.416838	4.200958	-2.652179
124.H	7.485252	3.316413	-0.342165
125.H	4.645411	5.914278	-0.473252
126.H	2.966164	-0.344821	-0.023419
127.H	4.951624	-1.634116	-0.297968
128.H	6.482143	-0.763741	-0.487957
129.P	10.127535	3.426084	-2.388460
130.O	11.654967	2.876744	-1.767790
131.O	9.942884	3.825540	-3.939380

132.O	9.142139	2.044712	-2.017945
133.C	9.325152	1.238123	-0.724333
134.C	9.453378	-0.252072	-1.036988
135.O	8.112499	-0.865478	-1.343054
136.C	10.325296	-0.644034	-2.250268
137.O	10.936424	-1.998142	-2.030757
138.C	9.337635	-0.649736	-3.440184
139.C	7.999498	-1.142172	-2.834636
140.N	6.801290	-0.480064	-3.315241
141.C	6.543621	0.896027	-3.284404
142.N	5.259274	1.165894	-3.410836
143.C	4.620459	-0.075253	-3.505768
144.C	3.239579	-0.411983	-3.499240
145.O	2.251518	0.370629	-3.443000
146.N	3.030203	-1.806882	-3.528637
147.C	4.039553	-2.754644	-3.569865
148.N	3.681744	-4.047770	-3.694239
149.N	5.343199	-2.436667	-3.498917
150.C	5.563195	-1.111644	-3.450496
151.H	8.416487	1.418671	-0.143739
152.H	10.220704	1.594619	-0.204728
153.H	9.804925	-0.734908	-0.116773
154.H	11.173020	0.031597	-2.393506
155.H	9.233716	0.366789	-3.833087
156.H	9.683266	-1.311331	-4.243905
157.H	7.848879	-2.219783	-2.937302
158.H	7.342178	1.608799	-3.128609
159.H	2.030373	-2.104426	-3.541836
160.H	2.700548	-4.388677	-3.651873
161.H	4.437209	-4.722581	-3.698459
162.H	-4.851546	-4.346281	-3.638236
163.H	-2.228757	-1.941885	-3.517653
164.P	-10.152861	-3.283089	-2.479824
165.O	-11.676531	-2.774321	-1.815670
166.O	-9.984833	-3.605210	-4.050437
167.O	-9.171381	-1.913827	-2.054865
168.H	-2.095113	-10.347681	3.775322
169.H	-2.215327	-11.407074	2.321712
170.H	-4.354500	-10.298458	2.580340
171.H	-1.967160	-7.927354	0.676913
172.H	-3.392168	-7.351953	-0.175662
173.H	-4.485638	-6.723532	1.953914
174.H	-0.731655	-7.402002	2.575577
175.C	-9.333082	-1.184174	-0.713502
176.H	-0.204888	-10.058002	2.345613
177.H	-2.961688	0.358880	0.020971
178.H	-2.763224	-1.262073	3.191590
179.H	-5.124287	-1.250702	3.081230
180.H	-5.964089	-2.781264	2.778495
181.P	-5.488707	-9.057899	-1.247187
182.O	-6.773321	-10.191096	-1.553085
183.O	-4.218935	-8.978184	-2.238301
184.H	-4.515700	-2.610418	-3.566420
185.O	-6.407467	-7.582856	-1.200645
186.C	-7.695956	-7.608416	-0.353528
187.C	-8.305443	-6.211729	-0.337468
188.O	-7.366548	-5.247559	0.351077
189.C	-8.599158	-5.571882	-1.711250
190.O	-9.750455	-4.595454	-1.367471
191.C	-7.320316	-4.799471	-2.031829
192.O	-5.065932	-9.396466	0.437788
193.H	-10.223483	-1.567247	-0.203984
194.N	-5.705136	-1.518002	-0.211223
195.C	-9.459972	0.322193	-0.935778
196.C	-9.370365	0.862233	-3.311662
197.C	-3.053993	-7.884858	0.712555
198.C	-6.944522	-4.205532	-0.657882
199.N	-5.544755	-3.928127	-0.484561
200.C	-4.474969	-4.816704	-0.567398

201.C	-10.344542	0.788287	-2.113031
202.H	-3.031814	-10.027937	0.153239
203.C	-8.024724	1.316406	-2.693438
204.N	-6.833053	0.683165	-3.226209
205.C	-6.576204	-0.692477	-3.277094
206.N	-3.315463	-4.204023	-0.426650
207.N	-5.293312	-0.954709	-3.431492
208.C	-4.654520	0.289659	-3.461440
209.C	-3.273358	0.625466	-3.448573
210.O	-2.285222	-0.158939	-3.445476
211.N	-3.063312	2.019721	-3.400354
212.C	-3.621868	-2.851737	-0.257768
213.C	-3.500855	-9.676806	2.285534
214.O	-3.649486	-8.355860	3.019976
215.O	-10.948743	2.128326	-1.805301
216.C	-3.564153	-9.319931	0.790952
217.C	-4.072447	2.968269	-3.376978
218.O	9.592977	-1.133082	2.225162
219.N	-3.715271	4.266419	-3.432755
220.C	10.311429	-2.299352	2.842230
221.C	9.630201	-3.586302	2.380103
222.O	8.292161	-3.761756	3.076539
223.N	-5.375463	2.646812	-3.311252
224.C	9.309915	-3.592934	0.876003
225.C	-5.595897	1.321183	-3.337537
226.H	-8.417783	-1.400717	-0.156236
227.O	9.399312	-5.079871	0.468270
228.C	2.864794	-3.607845	-0.317606
229.C	1.718190	-2.779436	-0.171005
230.O	1.675708	-1.525443	-0.092167
231.N	0.521843	-3.529241	-0.133905
232.C	0.441688	-4.909609	-0.266108
233.N	-0.768944	-5.483874	-0.298482
234.N	1.532462	-5.691958	-0.360866
235.C	2.674993	-4.995262	-0.400414
236.H	7.897186	-7.426390	0.588506
237.H	8.360890	-8.343342	-0.902265
238.H	6.269623	-9.221554	0.096644
239.H	6.326636	-8.864749	-2.633543
240.H	5.586145	-6.485554	-2.449664
241.H	4.105110	-7.342929	-2.958250
242.H	3.302677	-7.462705	-0.620153
243.H	5.891818	-4.616482	-0.771380
244.H	-0.350724	-2.956887	-0.079089
245.H	-1.647917	-4.936873	-0.353593
246.H	-0.784458	-6.461491	-0.611114
247.P	3.342514	-10.059879	-2.724644
248.O	2.813571	-11.600224	-2.118055
249.O	3.694196	-9.844196	-4.283150
250.O	1.970384	-9.085516	-2.293799
251.C	1.207335	-9.295113	-0.978105
252.C	-0.292546	-9.417559	-1.242948
253.O	-0.916177	-8.070665	-1.497990
254.C	-0.726441	-10.262708	-2.460851
255.O	-2.072392	-10.879307	-2.208180
256.C	-0.772759	-9.248914	-3.627649
257.C	-1.244287	-7.924960	-2.976186
258.N	-0.599125	-6.715933	-3.452854
259.C	0.777357	-6.458467	-3.465267
260.N	1.042954	-5.171500	-3.572918
261.C	-0.200484	-4.531262	-3.609606
262.C	-0.536429	-3.151010	-3.560716
263.O	0.247684	-2.163818	-3.509936
264.N	-1.931409	-2.941638	-3.536013
265.N	6.197769	-2.655057	2.578751
266.C	-1.184236	-6.421699	2.678647
267.C	-1.234590	-5.475497	-3.538243
268.H	1.407367	-8.398698	-0.385013
269.H	1.580270	-10.201383	-0.489510

270.H	-7.418027	-7.898380	0.665016
271.H	-0.743556	-9.788816	-0.314552
272.H	4.817960	4.563878	-3.436023
273.H	-8.379770	-8.332217	-0.806575
274.C	-3.515368	-7.223828	2.031283
275.H	-9.225748	-6.260287	0.259408
276.O	-8.120927	0.950146	-1.220290
277.H	-0.056500	-11.106704	-2.646280
278.C	-2.880361	-3.950357	-3.565327
279.N	-4.176844	-3.590748	-3.635932
280.N	-2.560437	-5.255102	-3.534116
281.H	0.229971	-9.135762	-4.052208
282.O	-1.054604	-9.633222	2.042667
283.H	-7.484596	-3.280944	-0.449602
284.C	7.876241	-3.081173	0.782215
285.N	-2.561673	-6.249158	2.531428
286.H	-4.647558	-5.868565	-0.740751
287.H	-2.324873	-7.772971	-3.037961
288.H	-8.949743	-6.263626	-2.481043
289.C	7.183850	-3.590686	2.066852
290.N	-0.572845	-5.285784	2.957061
291.C	-1.570388	-4.307749	2.982053
292.C	-1.506389	-2.892937	3.125155
293.O	-9.555556	1.021824	2.371034
294.C	-10.263523	2.151414	3.063435
295.C	-9.586432	3.462555	2.667468
296.O	-8.239547	3.597342	3.355613
297.C	-9.285033	3.556444	1.162401
298.O	-9.375393	5.065258	0.843109
299.C	-7.854277	3.047348	1.020826
300.C	-7.144213	3.478103	2.324436
301.N	-6.156172	2.510637	2.769721
302.C	-6.325239	1.129760	2.887667
303.N	-5.182128	0.511611	3.117555
304.C	-4.203081	1.508225	3.139139
305.C	-2.784902	1.440867	3.242115
306.O	-2.057457	0.403539	3.318395
307.N	-2.191644	2.713573	3.236593
308.C	-2.886262	3.913043	3.142814
309.N	-2.185270	5.056198	3.259287
310.N	-4.214661	3.972964	2.966601
311.C	-4.801526	2.767225	2.956298
312.H	-10.199555	2.025599	4.152104
313.H	-11.315540	2.176867	2.744447
314.H	-10.196394	4.309777	3.002409
315.H	-10.016369	3.036800	0.540655
316.H	-7.900432	1.961705	0.961804
317.H	-7.353344	3.404649	0.121588
318.H	-6.642319	4.447722	2.249635
319.H	-7.308473	0.679825	2.803034
320.H	-1.152402	2.695990	3.297927
321.H	-1.142956	5.058247	3.248144
322.H	-2.680344	5.906157	3.009843
323.P	-9.094408	5.523688	-0.843080
324.O	-10.234391	6.814710	-1.089557
325.O	-9.047916	4.274576	-1.862258
326.O	-7.617884	6.441562	-0.818931
327.C	-7.618969	7.708673	0.060373
328.C	-6.222939	8.320086	0.050152
329.O	-5.237489	7.366304	0.685649
330.C	-5.625232	8.649598	-1.334566
331.O	-4.641526	9.795493	-0.992412
332.C	-4.861916	7.380078	-1.710207
333.C	-4.226919	6.969557	-0.364855
334.N	-3.945397	5.565726	-0.235177
335.C	-4.836385	4.498022	-0.320300
336.N	-4.220708	3.335358	-0.225648
337.C	-2.864140	3.637742	-0.086464
338.C	-1.717359	2.801142	-0.000089

339.O	-1.675952	1.544690	0.004469
340.N	-0.519299	3.546172	0.068296
341.C	-0.438233	4.931672	0.013187
342.N	0.772569	5.505821	-0.003635
343.N	-1.528680	5.719342	-0.023290
344.C	-2.672653	5.027519	-0.091152
345.H	-7.878790	7.405342	1.079827
346.H	-8.356186	8.402482	-0.354321
347.H	-6.254886	9.225125	0.671069
348.H	-6.340725	9.017319	-2.074107
349.H	-5.598612	6.634172	-2.030079
350.H	-4.121487	7.517756	-2.503595
351.H	-3.296080	7.504103	-0.171084
352.H	-5.892446	4.674671	-0.460768
353.H	0.352910	2.970992	0.080003
354.H	1.650303	4.962679	-0.099987
355.H	0.784820	6.500208	-0.257990
356.P	-3.357410	10.223055	-2.128655
357.O	-2.822637	11.726324	-1.439665
358.O	-3.720862	10.096396	-3.694163
359.O	-1.984676	9.223385	-1.762475
360.C	-1.211875	9.354872	-0.442207
361.C	0.286404	9.489561	-0.710675
362.O	0.905113	8.158511	-1.047634
363.C	0.711822	10.402077	-1.882058
364.O	2.061758	10.999377	-1.606776
365.C	0.744287	9.456357	-3.105138
366.C	1.219549	8.096913	-2.534694
367.N	0.568415	6.917383	-3.073027
368.C	-0.808197	6.660400	-3.084046
369.N	-1.075283	5.381450	-3.260969
370.C	0.167621	4.744895	-3.348358
371.C	0.503918	3.364213	-3.382027
372.O	-0.279719	2.375479	-3.378467
373.N	1.899113	3.154505	-3.385431
374.C	2.847714	4.163768	-3.368810
375.N	4.143302	3.809343	-3.476195
376.N	2.528328	5.464466	-3.260345
377.C	1.202541	5.683996	-3.235935
378.H	-1.409130	8.425654	0.098958
379.H	-1.579693	10.231534	0.101248
380.H	0.746089	9.806685	0.233534
381.H	0.042552	11.256953	-2.012229
382.H	-0.262913	9.368830	-3.525013
383.H	1.425493	9.827658	-3.880552
384.H	2.299260	7.947676	-2.615443
385.H	-1.524177	7.454113	-2.918173
386.H	2.196383	2.155242	-3.423125
387.H	4.482623	2.826790	-3.456200
388.H	10.230436	-2.715642	-2.115571
389.H	-10.242074	2.848179	-1.857013
390.H	-2.791830	-10.171381	-2.248468
391.H	-1.461276	-9.577028	-4.415933
392.H	2.779210	10.294257	-1.699638
393.H	-11.192647	6.518695	-1.173494
394.H	-3.494997	12.472844	-1.489593
395.H	6.472952	11.231964	-1.138011
396.H	-9.968784	0.165947	2.672649
397.H	-6.480223	-11.152151	-1.612588
398.H	12.398932	3.551083	-1.828665
399.H	0.253976	9.909241	2.914698
400.H	10.008884	-0.295230	2.570639
401.K	-0.008884	0.056182	-1.710494
402.Li	0.019649	-0.087894	3.134798

Table S20 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K⁺–Na⁺** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–K^+–Na^+ (Bond Energy: -55751.71 kcal/mol)

1.C	6.478625	-1.278845	2.780873
2.N	5.340066	-0.663881	3.040593
3.C	4.359121	-1.659320	3.026758
4.C	2.940950	-1.579027	3.102400
5.O	2.224423	-0.540144	3.177470
6.N	2.331794	-2.848036	3.050534
7.C	3.013585	-4.047131	2.902439
8.N	2.299031	-5.189364	2.948315
9.N	4.343654	-4.112617	2.732621
10.C	4.945254	-2.912848	2.787650
11.H	10.396041	-2.243849	3.884416
12.H	11.462483	-2.320913	2.432874
13.H	10.344702	-4.463777	2.613830
14.H	10.085572	-3.048891	0.234923
15.H	7.976471	-2.014611	0.772274
16.H	7.409532	-3.421306	-0.116340
17.H	6.771169	-4.565047	1.979394
18.H	7.464718	-0.832887	2.709032
19.H	1.290065	-2.833894	3.099416
20.H	1.258762	-5.207519	2.939704
21.H	2.796482	-6.032780	2.681839
22.P	9.093749	-5.448430	-1.256928
23.O	10.179779	-6.757746	-1.618810
24.O	9.041270	-4.144932	-2.204902
25.O	7.590092	-6.321843	-1.218257
26.C	7.586792	-7.625611	-0.394160
27.C	-2.784087	-1.628352	-0.027778
28.C	6.191289	-8.233938	-0.438898
29.O	5.205755	-7.313741	0.246126
30.C	5.597076	-8.485504	-1.841014
31.O	4.618158	-9.652340	-1.566725
32.C	4.828091	-7.200064	-2.145266
33.C	4.190122	-6.872070	-0.779333
34.H	-2.725721	4.610768	-3.367872
35.N	3.893551	-5.480310	-0.568569
36.H	-4.462704	4.950576	-3.406586
37.H	-4.961044	1.706810	-0.139210
38.N	-3.543554	-0.444354	0.030699
39.N	-5.070048	-2.354410	3.070827
40.H	-6.497205	0.840192	-0.397143
41.C	-4.927959	-0.374901	-0.095503
42.H	-6.522048	-5.502755	-2.330813
43.O	-1.525327	-1.572487	0.083625
44.H	-7.400211	-4.018472	-2.794679
45.H	-9.812907	0.768471	-0.000413
46.H	-11.200762	0.137634	-2.306978
47.H	-9.274485	-0.116309	-3.777629
48.H	-9.724173	1.583224	-4.088346
49.H	-7.879468	2.413794	-2.744919
50.H	1.479565	-7.264420	-3.382927
51.C	4.771268	-4.400438	-0.576632
52.N	4.142506	-3.255476	-0.395395
53.O	-0.415593	-2.281957	3.132880
54.C	-3.930295	-3.067328	2.969236
55.C	-2.205362	-10.472464	2.621976
56.N	-2.726525	-2.388363	3.088640
57.H	-12.386254	-3.486513	-1.898254
58.H	-7.382467	-1.396957	-3.177025
59.C	-4.987672	-2.603632	-0.280665
60.H	-2.063047	2.323154	-3.370920
61.H	3.533083	-12.302771	-2.222345
62.H	11.143743	-6.488021	-1.721832
63.N	-4.002163	-4.393567	2.774497
64.C	-2.801250	-4.995341	2.771516
65.N	-5.512556	0.827438	-0.105912
66.O	1.104758	9.589750	2.539712
67.C	2.252613	10.290936	3.208634

68.C	3.551473	9.618950	2.767319
69.O	3.707489	8.266443	3.439720
70.C	3.598580	9.332049	1.257095
71.O	5.093589	9.438604	0.886750
72.C	3.096379	7.898311	1.117139
73.C	3.561367	7.179409	2.404545
74.N	2.603929	6.188086	2.863784
75.C	1.223800	6.360208	3.011395
76.N	0.603320	5.213983	3.218919
77.C	1.599095	4.233627	3.196684
78.C	1.517689	2.813960	3.225793
79.O	0.477315	2.095993	3.252363
80.N	2.787829	2.206458	3.186470
81.C	3.989814	2.892344	3.089324
82.N	5.130912	2.176568	3.141410
83.N	4.058840	4.227049	2.962099
84.C	2.857770	4.826829	3.006970
85.H	2.157363	10.214280	4.299506
86.H	2.268246	11.346429	2.901024
87.H	4.408338	10.226491	3.081617
88.H	3.052612	10.064932	0.660251
89.H	2.009356	7.935074	1.081925
90.H	3.438826	7.406334	0.206664
91.H	4.528505	6.677404	2.300397
92.H	0.779323	7.348316	2.962272
93.H	2.773404	1.163606	3.204723
94.H	5.150125	1.137018	3.102106
95.H	5.980293	2.681648	2.910555
96.P	5.492108	9.136719	-0.811463
97.O	6.807653	10.237847	-1.095834
98.O	4.213950	9.118744	-1.794715
99.O	6.365499	7.633102	-0.810086
100.C	7.644053	7.592862	0.051336
101.C	8.251034	6.198652	-0.033949
102.O	7.312566	5.189565	0.588903
103.C	8.535704	5.659865	-1.452412
104.O	9.696658	4.670777	-1.190253
105.C	7.257565	4.904928	-1.817500
106.C	6.895391	4.215092	-0.485873
107.N	5.498915	3.912361	-0.320756
108.C	4.419083	4.790112	-0.329847
109.N	3.270362	4.156684	-0.194785
110.C	3.591359	2.799701	-0.107252
111.C	2.783251	1.639528	0.034990
112.O	1.525764	1.576946	0.156189
113.N	3.544555	0.455138	0.026140
114.C	4.928390	0.394638	-0.113491
115.N	5.514365	-0.804781	-0.189743
116.N	5.694324	1.498391	-0.172970
117.C	4.983819	2.630020	-0.186222
118.H	7.354085	7.806562	1.085114
119.H	8.335186	8.346516	-0.337675
120.H	9.174431	6.202385	0.559979
121.H	8.873940	6.407470	-2.173951
122.H	6.498853	5.649711	-2.083764
123.H	7.373726	4.197674	-2.643779
124.H	7.444590	3.282939	-0.345194
125.H	4.571876	5.852638	-0.450940
126.H	2.974979	-0.417959	0.067746
127.H	4.961464	-1.680557	-0.268708
128.H	6.495721	-0.800780	-0.492077
129.P	10.090547	3.437307	-2.392379
130.O	11.633149	2.905432	-1.794611
131.O	9.881268	3.854304	-3.935319
132.O	9.133187	2.034591	-2.029072
133.C	9.333453	1.227914	-0.738482
134.C	9.462207	-0.261333	-1.054215
135.O	8.120658	-0.877196	-1.354862
136.C	10.328964	-0.650226	-2.272051

137.O	10.942922	-2.003900	-2.057160
138.C	9.336396	-0.655988	-3.457583
139.C	8.002265	-1.151963	-2.846857
140.N	6.801102	-0.490796	-3.320793
141.C	6.545532	0.885925	-3.296710
142.N	5.260558	1.156865	-3.412000
143.C	4.619529	-0.084037	-3.492412
144.C	3.239869	-0.419173	-3.464481
145.O	2.253782	0.366382	-3.392774
146.N	3.026721	-1.813105	-3.486537
147.C	4.034409	-2.763140	-3.536048
148.N	3.673347	-4.055528	-3.643325
149.N	5.339129	-2.446469	-3.476489
150.C	5.561648	-1.121608	-3.440450
151.H	8.432658	1.405446	-0.144938
152.H	10.234797	1.585760	-0.229887
153.H	9.819936	-0.744352	-0.136412
154.H	11.174913	0.027039	-2.418340
155.H	9.229276	0.361004	-3.848264
156.H	9.679594	-1.315685	-4.263861
157.H	7.853191	-2.229671	-2.949993
158.H	7.346398	1.598660	-3.154038
159.H	2.027136	-2.110107	-3.500784
160.H	2.690064	-4.392628	-3.638464
161.H	4.426803	-4.728945	-3.711039
162.H	-4.861280	-4.334470	-3.659376
163.H	-2.235778	-1.939380	-3.479287
164.P	-10.126756	-3.284039	-2.481926
165.O	-11.661789	-2.791709	-1.832131
166.O	-9.942019	-3.620157	-4.047653
167.O	-9.169161	-1.896143	-2.063373
168.H	-2.095383	-10.474936	3.714233
169.H	-2.229731	-11.503200	2.239629
170.H	-4.362484	-10.389120	2.535054
171.H	-1.984055	-7.980425	0.654722
172.H	-3.423399	-7.391277	-0.164919
173.H	-4.484138	-6.803206	1.988643
174.H	-0.726508	-7.511218	2.558234
175.C	-9.344658	-1.166397	-0.724287
176.H	-0.213311	-10.160178	2.281549
177.H	-2.972963	0.425074	0.114833
178.H	-2.711016	-1.347902	3.159386
179.H	-5.089215	-1.314189	3.081785
180.H	-5.922551	-2.847068	2.825155
181.P	-5.498690	-9.056303	-1.265525
182.O	-6.814372	-10.145672	-1.594696
183.O	-4.231567	-8.981895	-2.260325
184.H	-4.522323	-2.599789	-3.555784
185.O	-6.376535	-7.558116	-1.175107
186.C	-7.652660	-7.571380	-0.309199
187.C	-8.258584	-6.174196	-0.304780
188.O	-7.314009	-5.205376	0.370690
189.C	-8.554221	-5.549687	-1.685165
190.O	-9.710181	-4.576588	-1.351902
191.C	-7.278155	-4.775169	-2.014241
192.O	-5.079190	-9.452783	0.408433
193.H	-10.241051	-1.548489	-0.224559
194.N	-5.696154	-1.473142	-0.206155
195.C	-9.470206	0.339246	-0.949934
196.C	-9.373231	0.876331	-3.326605
197.C	-3.070352	-7.942609	0.706751
198.C	-6.904556	-4.167830	-0.646004
199.N	-5.506216	-3.876899	-0.473788
200.C	-4.428191	-4.754700	-0.536301
201.C	-10.350966	0.802850	-2.131001
202.H	-3.045922	-10.075007	0.107657
203.C	-8.030100	1.332015	-2.704692
204.N	-6.836556	0.698333	-3.232657
205.C	-6.582354	-0.677721	-3.288710

206.N	-3.277124	-4.130559	-0.379463
207.N	-5.299012	-0.942409	-3.433631
208.C	-4.657416	0.300727	-3.451946
209.C	-3.277059	0.633387	-3.419107
210.O	-2.290720	-0.154799	-3.399998
211.N	-3.062767	2.026279	-3.365726
212.C	-3.594873	-2.779028	-0.221678
213.C	-3.507118	-9.766335	2.247604
214.O	-3.642326	-8.460120	3.010289
215.O	-10.957945	2.142427	-1.827314
216.C	-3.577525	-9.380230	0.760420
217.C	-4.069934	2.977930	-3.350536
218.O	9.693451	-1.146534	2.182284
219.N	-3.708951	4.274262	-3.390238
220.C	10.422230	-2.311665	2.789050
221.C	9.727600	-3.597988	2.346225
222.O	8.403862	-3.765301	3.071629
223.N	-5.374211	2.658837	-3.294794
224.C	9.377296	-3.608513	0.848570
225.C	-5.597731	1.334123	-3.331346
226.H	-8.436769	-1.382634	-0.154949
227.O	9.464625	-5.094223	0.437708
228.C	2.788331	-3.578888	-0.277420
229.C	1.633205	-2.775234	-0.080804
230.O	1.574685	-1.520902	0.072103
231.N	0.448842	-3.536419	-0.073027
232.C	0.383599	-4.916302	-0.245014
233.N	-0.817758	-5.500690	-0.298738
234.N	1.484705	-5.680023	-0.357708
235.C	2.615811	-4.969041	-0.385805
236.H	7.842822	-7.365532	0.637989
237.H	8.324561	-8.303015	-0.834282
238.H	6.220025	-9.171356	0.131936
239.H	6.315365	-8.806326	-2.599392
240.H	5.561465	-6.433573	-2.420873
241.H	4.089256	-7.296859	-2.946079
242.H	3.264325	-7.425944	-0.616287
243.H	5.829912	-4.550858	-0.730433
244.H	-0.422481	-2.968631	0.010208
245.H	-1.696261	-4.947557	-0.331899
246.H	-0.824130	-6.474644	-0.624057
247.P	3.346765	-10.024653	-2.735614
248.O	2.836592	-11.580362	-2.152838
249.O	3.714828	-9.783907	-4.286473
250.O	1.953281	-9.078645	-2.311222
251.C	1.189134	-9.306401	-0.999791
252.C	-0.309618	-9.427196	-1.269790
253.O	-0.933093	-8.078746	-1.519966
254.C	-0.740009	-10.266550	-2.492826
255.O	-2.085892	-10.885647	-2.246124
256.C	-0.784896	-9.247751	-3.655084
257.C	-1.259141	-7.927652	-2.998556
258.N	-0.613966	-6.715908	-3.468048
259.C	0.763030	-6.460573	-3.483746
260.N	1.030672	-5.173132	-3.577329
261.C	-0.211913	-4.530661	-3.601023
262.C	-0.545342	-3.152317	-3.526680
263.O	0.242355	-2.167863	-3.455888
264.N	-1.939137	-2.938997	-3.496781
265.N	6.301383	-2.655246	2.606644
266.C	-1.169077	-6.527178	2.668827
267.C	-1.247669	-5.474115	-3.536978
268.H	1.387218	-8.419455	-0.392072
269.H	1.561489	-10.219466	-0.523522
270.H	-7.360051	-7.849708	0.708366
271.H	-0.762304	-9.804179	-0.344545
272.H	4.824978	4.555442	-3.459392
273.H	-8.345134	-8.298671	-0.743208
274.C	-3.514820	-7.308634	2.044875

275.H	-9.177059	-6.213089	0.295419
276.O	-8.130006	0.967294	-1.231007
277.H	-0.068687	-11.108875	-2.680972
278.C	-2.890809	-3.945461	-3.538535
279.N	-4.186010	-3.582663	-3.591534
280.N	-2.572848	-5.251169	-3.521952
281.H	0.218566	-9.132166	-4.077167
282.O	-1.063524	-9.728437	1.990143
283.H	-7.451467	-3.245535	-0.444482
284.C	7.939748	-3.102192	0.781147
285.N	-2.551049	-6.346903	2.551034
286.H	-4.584912	-5.809746	-0.707721
287.H	-2.339787	-7.776644	-3.061145
288.H	-8.900195	-6.251370	-2.448026
289.C	7.275021	-3.599081	2.085622
290.N	-0.544342	-5.394232	2.929992
291.C	-1.539435	-4.413750	2.975785
292.C	-1.456540	-2.997574	3.080121
293.O	-9.643456	1.030413	2.339007
294.C	-10.361781	2.158649	3.022620
295.C	-9.670897	3.468367	2.647180
296.O	-8.337135	3.591216	3.362617
297.C	-9.340849	3.568128	1.148305
298.O	-9.426854	5.076737	0.829448
299.C	-7.906751	3.061922	1.030851
300.C	-7.222278	3.478396	2.353071
301.N	-6.245159	2.502905	2.805033
302.C	-6.422153	1.118604	2.898979
303.N	-5.281772	0.488672	3.110724
304.C	-4.299906	1.482756	3.146974
305.C	-2.881192	1.397988	3.205578
306.O	-2.164361	0.356522	3.212602
307.N	-2.271596	2.667545	3.224587
308.C	-2.953714	3.873495	3.153147
309.N	-2.237468	5.010538	3.258793
310.N	-4.285152	3.949304	2.999611
311.C	-4.887183	2.748573	2.988424
312.H	-10.320922	2.026792	4.111681
313.H	-11.406762	2.189926	2.681825
314.H	-10.282880	4.317172	2.974466
315.H	-10.059731	3.049072	0.511746
316.H	-7.948329	1.976994	0.957742
317.H	-7.387987	3.432435	0.146622
318.H	-6.716089	4.447330	2.297152
319.H	-7.409375	0.678213	2.810497
320.H	-1.229581	2.650320	3.264331
321.H	-1.197179	5.028067	3.240513
322.H	-2.736053	5.868425	3.045956
323.P	-9.094872	5.531434	-0.849259
324.O	-10.199173	6.848660	-1.115582
325.O	-9.053916	4.284303	-1.870917
326.O	-7.596892	6.411909	-0.791559
327.C	-7.581374	7.665603	0.106303
328.C	-6.184562	8.272185	0.079641
329.O	-5.194757	7.311740	0.700124
330.C	-5.605156	8.601183	-1.312966
331.O	-4.622944	9.751315	-0.984491
332.C	-4.842391	7.333428	-1.697677
333.C	-4.191520	6.925988	-0.359580
334.N	-3.896735	5.523553	-0.230629
335.C	-4.776575	4.447087	-0.293053
336.N	-4.149057	3.292572	-0.180940
337.C	-2.793370	3.606503	-0.054214
338.C	-1.637961	2.791233	0.087017
339.O	-1.579423	1.530370	0.168687
340.N	-0.452127	3.549335	0.128202
341.C	-0.385718	4.936555	0.033089
342.N	0.815932	5.521588	0.000898
343.N	-1.486390	5.706939	-0.026258

344.C	-2.618879	5.000422	-0.085297
345.H	-7.825866	7.347386	1.124883
346.H	-8.322604	8.368383	-0.285671
347.H	-6.203783	9.176017	0.702685
348.H	-6.331525	8.964434	-2.044074
349.H	-5.580947	6.585778	-2.008805
350.H	-4.111750	7.474262	-2.499444
351.H	-3.262452	7.467194	-0.174958
352.H	-5.835800	4.607482	-0.431759
353.H	0.418872	2.976942	0.171710
354.H	1.692706	4.970114	-0.076353
355.H	0.820178	6.512902	-0.267171
356.P	-3.359546	10.189755	-2.139244
357.O	-2.840993	11.707386	-1.469725
358.O	-3.736929	10.041426	-3.699424
359.O	-1.968584	9.215004	-1.776766
360.C	-1.197118	9.360052	-0.457755
361.C	0.300301	9.496543	-0.728387
362.O	0.921682	8.165619	-1.063131
363.C	0.722223	10.407203	-1.902420
364.O	2.070352	11.009533	-1.629674
365.C	0.756312	9.459310	-3.123687
366.C	1.233334	8.101701	-2.551074
367.N	0.581364	6.920700	-3.085346
368.C	-0.795974	6.666758	-3.101935
369.N	-1.065436	5.387044	-3.268194
370.C	0.176450	4.747008	-3.342828
371.C	0.509908	3.366531	-3.354556
372.O	-0.277291	2.379465	-3.333176
373.N	1.903900	3.152214	-3.353216
374.C	2.855481	4.159593	-3.346697
375.N	4.149543	3.800930	-3.441189
376.N	2.538474	5.461892	-3.248609
377.C	1.213296	5.684995	-3.234479
378.H	-1.392216	8.436502	0.093713
379.H	-1.566430	10.241300	0.077288
380.H	0.759845	9.817602	0.214535
381.H	0.050040	11.259553	-2.034278
382.H	-0.250565	9.370141	-3.543854
383.H	1.437268	9.830132	-3.899519
384.H	2.312970	7.952885	-2.633000
385.H	-1.510957	7.463574	-2.948091
386.H	2.200108	2.153020	-3.390970
387.H	4.486378	2.817402	-3.450215
388.H	10.237724	-2.722338	-2.140688
389.H	-10.251622	2.862972	-1.875864
390.H	-2.805928	-10.178048	-2.282504
391.H	-1.471603	-9.572860	-4.446148
392.H	2.790307	10.306720	-1.721013
393.H	-11.162718	6.574940	-1.214794
394.H	-3.524700	12.443470	-1.521473
395.H	6.539613	11.205769	-1.160224
396.H	-10.064805	0.174216	2.628090
397.H	-6.546688	-11.111642	-1.685365
398.H	12.364007	3.594447	-1.849449
399.H	0.257112	9.996893	2.871369
400.H	10.115522	-0.308005	2.518449
401.K	-0.011617	0.059181	-1.781252
402.Na	0.017975	-0.052271	1.900178

Table S21 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K$^+$–K$^+$** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–K$^+$–K$^+$ (Bond Energy: -55756.14 kcal/mol)			
1.C	6.516361	-1.317680	2.807133
2.N	5.395243	-0.699408	3.128807
3.C	4.405401	-1.686146	3.113255

4.C	2.998096	-1.594360	3.284005
5.O	2.307057	-0.554854	3.476254
6.N	2.364116	-2.851960	3.186146
7.C	3.020964	-4.050598	2.945458
8.N	2.288559	-5.183615	2.954027
9.N	4.342703	-4.125361	2.723129
10.C	4.964774	-2.936031	2.803470
11.H	10.395706	-2.312478	3.880441
12.H	11.474916	-2.378823	2.437827
13.H	10.347059	-4.515451	2.575859
14.H	10.101547	-3.065753	0.217233
15.H	7.996102	-2.028866	0.763112
16.H	7.425519	-3.418078	-0.149053
17.H	6.769119	-4.588663	1.928074
18.H	7.505551	-0.881418	2.718854
19.H	1.329715	-2.842511	3.303777
20.H	1.250973	-5.200356	2.992696
21.H	2.764554	-6.021290	2.635880
22.P	9.104574	-5.450306	-1.305041
23.O	10.199942	-6.747164	-1.683057
24.O	9.041684	-4.136763	-2.238437
25.O	7.608380	-6.336513	-1.271386
26.C	7.619030	-7.644968	-0.454377
27.C	-2.794860	-1.665711	-0.045385
28.C	6.223596	-8.254146	-0.480642
29.O	5.247811	-7.335511	0.220851
30.C	5.609253	-8.502187	-1.874583
31.O	4.633580	-9.668903	-1.589245
32.C	4.836531	-7.215659	-2.164474
33.C	4.218067	-6.891606	-0.788503
34.H	-2.731510	4.608234	-3.366235
35.N	3.925685	-5.499405	-0.570903
36.H	-4.469067	4.946103	-3.397437
37.H	-4.968760	1.680471	-0.118458
38.N	-3.549333	-0.477868	0.025838
39.N	-5.072109	-2.354187	3.084420
40.H	-6.502256	0.817197	-0.365618
41.C	-4.935354	-0.404730	-0.080618
42.H	-6.529872	-5.501523	-2.352744
43.O	-1.533283	-1.612058	0.037773
44.H	-7.405262	-4.010191	-2.798584
45.H	-9.823737	0.759895	0.006302
46.H	-11.204449	0.136864	-2.307131
47.H	-9.271712	-0.121482	-3.768779
48.H	-9.714728	1.579618	-4.080132
49.H	-7.876595	2.403239	-2.723183
50.H	1.492459	-7.261950	-3.369071
51.C	4.806048	-4.420614	-0.586777
52.N	4.182154	-3.272720	-0.407465
53.O	-0.427318	-2.380469	3.435284
54.C	-3.940075	-3.085416	3.018059
55.C	-2.264143	-10.488913	2.611692
56.N	-2.733556	-2.433460	3.230268
57.H	-12.393882	-3.496703	-1.918664
58.H	-7.378099	-1.406086	-3.157394
59.C	-5.001608	-2.634504	-0.270083
60.H	-2.065535	2.322274	-3.384910
61.H	3.530042	-12.319091	-2.236997
62.H	11.161946	-6.469534	-1.783812
63.N	-4.022851	-4.401698	2.768243
64.C	-2.831235	-5.024250	2.789223
65.N	-5.517186	0.800655	-0.074906
66.O	1.144117	9.623036	2.528043
67.C	2.304978	10.313513	3.185587
68.C	3.593959	9.633753	2.727565
69.O	3.754948	8.281408	3.398828
70.C	3.619699	9.344722	1.217551
71.O	5.110856	9.444799	0.831155
72.C	3.109068	7.912870	1.085763

73.C	3.587092	7.192761	2.367518
74.N	2.628871	6.212011	2.846195
75.C	1.256087	6.405753	3.035524
76.N	0.629934	5.275918	3.307557
77.C	1.616929	4.286425	3.287785
78.C	1.521314	2.875169	3.418029
79.O	0.477456	2.179673	3.566139
80.N	2.780988	2.243518	3.333298
81.C	3.985173	2.906269	3.141197
82.N	5.117548	2.172917	3.156217
83.N	4.065474	4.233899	2.959480
84.C	2.874274	4.854053	3.027073
85.H	2.221575	10.235146	4.277331
86.H	2.325220	11.369650	2.880154
87.H	4.457868	10.237866	3.028791
88.H	3.069325	10.078847	0.626235
89.H	2.021854	7.955410	1.064838
90.H	3.436044	7.419111	0.170630
91.H	4.549188	6.683804	2.251968
92.H	0.822113	7.397437	2.966444
93.H	2.768986	1.205978	3.418536
94.H	5.133145	1.134611	3.161912
95.H	5.962508	2.657168	2.871401
96.P	5.494450	9.147524	-0.870431
97.O	6.798009	10.259413	-1.168187
98.O	4.205689	9.120052	-1.839527
99.O	6.381571	7.651577	-0.873779
100.C	7.668295	7.629151	-0.023263
101.C	8.275552	6.233959	-0.084454
102.O	7.339600	5.236135	0.560572
103.C	8.555810	5.668667	-1.493241
104.O	9.717576	4.684940	-1.216015
105.C	7.276623	4.906790	-1.839549
106.C	6.919814	4.241558	-0.493799
107.N	5.522952	3.942529	-0.318912
108.C	4.444461	4.823220	-0.336103
109.N	3.292784	4.195018	-0.201869
110.C	3.612527	2.837998	-0.106598
111.C	2.800194	1.681345	0.014831
112.O	1.539635	1.622879	0.108587
113.N	3.555620	0.491948	0.016384
114.C	4.940916	0.425758	-0.104327
115.N	5.523148	-0.778013	-0.165886
116.N	5.710588	1.527003	-0.159981
117.C	5.004819	2.662464	-0.179295
118.H	7.388116	7.864524	1.008555
119.H	8.354956	8.374768	-0.434861
120.H	9.200903	6.249208	0.506255
121.H	8.891328	6.402684	-2.229879
122.H	6.516535	5.646542	-2.115840
123.H	7.389476	4.184746	-2.653351
124.H	7.469684	3.312082	-0.338028
125.H	4.602865	5.884309	-0.462235
126.H	2.988331	-0.382982	0.034226
127.H	4.973175	-1.653455	-0.256067
128.H	6.504949	-0.778731	-0.468109
129.P	10.111141	3.433118	-2.398919
130.O	11.649235	2.903699	-1.788389
131.O	9.908504	3.829981	-3.948122
132.O	9.145639	2.040234	-2.019852
133.C	9.351946	1.234772	-0.729422
134.C	9.472558	-0.254954	-1.045843
135.O	8.126444	-0.862275	-1.344580
136.C	10.335204	-0.645575	-2.266479
137.O	10.945901	-2.001185	-2.054717
138.C	9.339821	-0.647639	-3.449447
139.C	8.006439	-1.141336	-2.835592
140.N	6.805167	-0.481025	-3.309576
141.C	6.547710	0.895061	-3.283220

142.N	5.262784	1.164592	-3.403623
143.C	4.624231	-0.077276	-3.490349
144.C	3.245142	-0.414711	-3.474647
145.O	2.257413	0.369646	-3.411459
146.N	3.034169	-1.808880	-3.498827
147.C	4.043578	-2.757523	-3.543038
148.N	3.684617	-4.050477	-3.652328
149.N	5.347327	-2.438751	-3.476975
150.C	5.567552	-1.113655	-3.436416
151.H	8.456198	1.417624	-0.129847
152.H	10.258244	1.589677	-0.227716
153.H	9.830331	-0.741950	-0.129946
154.H	11.182580	0.029686	-2.413895
155.H	9.233558	0.369917	-3.838802
156.H	9.679215	-1.307070	-4.257575
157.H	7.856896	-2.219142	-2.936979
158.H	7.347368	1.608065	-3.134931
159.H	2.035315	-2.107314	-3.519931
160.H	2.702012	-4.389052	-3.645397
161.H	4.439152	-4.723397	-3.712843
162.H	-4.853147	-4.342409	-3.651081
163.H	-2.230761	-1.942813	-3.496278
164.P	-10.133665	-3.285814	-2.496096
165.O	-11.672093	-2.799318	-1.850323
166.O	-9.939860	-3.607394	-4.063752
167.O	-9.177309	-1.902442	-2.060191
168.H	-2.168566	-10.483504	3.705292
169.H	-2.288915	-11.522419	2.236961
170.H	-4.418774	-10.400268	2.488910
171.H	-2.002930	-8.003277	0.640702
172.H	-3.426054	-7.410700	-0.202456
173.H	-4.515730	-6.807965	1.933874
174.H	-0.780600	-7.559575	2.563418
175.C	-9.363896	-1.177773	-0.719924
176.H	-0.266123	-10.195005	2.290321
177.H	-2.981642	0.394802	0.087805
178.H	-2.720315	-1.401917	3.370877
179.H	-5.087622	-1.317428	3.141205
180.H	-5.920395	-2.823914	2.785493
181.P	-5.501629	-9.064844	-1.321584
182.O	-6.807605	-10.158414	-1.673715
183.O	-4.222684	-8.978655	-2.300234
184.H	-4.516272	-2.607107	-3.554463
185.O	-6.388754	-7.572299	-1.228756
186.C	-7.670103	-7.600473	-0.370458
187.C	-8.276459	-6.203861	-0.346693
188.O	-7.334377	-5.245900	0.348267
189.C	-8.565235	-5.558109	-1.718570
190.O	-9.722308	-4.589553	-1.377036
191.C	-7.287568	-4.778714	-2.029227
192.O	-5.099968	-9.466762	0.354391
193.H	-10.267752	-1.557299	-0.231775
194.N	-5.706272	-1.501204	-0.188123
195.C	-9.479379	0.329153	-0.942150
196.C	-9.369955	0.870927	-3.317209
197.C	-3.089747	-7.960782	0.676601
198.C	-6.920907	-4.192810	-0.649699
199.N	-5.522351	-3.905534	-0.468076
200.C	-4.445154	-4.785001	-0.539937
201.C	-10.353118	0.798866	-2.126385
202.H	-3.063927	-10.094686	0.082155
203.C	-8.028634	1.321460	-2.688044
204.N	-6.834587	0.689194	-3.215573
205.C	-6.578965	-0.686282	-3.272653
206.N	-3.291582	-4.165187	-0.384845
207.N	-5.295763	-0.949255	-3.423011
208.C	-4.656420	0.295056	-3.444618
209.C	-3.276749	0.630514	-3.426024
210.O	-2.288919	-0.156186	-3.419234

211.N	-3.064477	2.023651	-3.372422
212.C	-3.608905	-2.814344	-0.218804
213.C	-3.557508	-9.779893	2.214369
214.O	-3.705548	-8.471423	2.970695
215.O	-10.956322	2.140308	-1.823038
216.C	-3.602928	-9.396999	0.725767
217.C	-4.073232	2.973741	-3.348351
218.O	9.716691	-1.189442	2.185327
219.N	-3.714356	4.270724	-3.387224
220.C	10.431530	-2.367042	2.784602
221.C	9.733586	-3.643765	2.319448
222.O	8.406603	-3.820663	3.036293
223.N	-5.376404	2.652191	-3.285282
224.C	9.388690	-3.630565	0.820921
225.C	-5.597669	1.327095	-3.319793
226.H	-8.463662	-1.401429	-0.141322
227.O	9.471852	-5.111574	0.392641
228.C	2.828175	-3.595247	-0.282609
229.C	1.675825	-2.787088	-0.106930
230.O	1.620376	-1.529076	0.018099
231.N	0.486976	-3.543138	-0.087259
232.C	0.416921	-4.925234	-0.238946
233.N	-0.788061	-5.506754	-0.275749
234.N	1.515877	-5.692284	-0.348714
235.C	2.650301	-4.985391	-0.383898
236.H	7.890700	-7.390410	0.575153
237.H	8.350725	-8.318755	-0.909830
238.H	6.260682	-9.192857	0.087547
239.H	6.316591	-8.821257	-2.643897
240.H	5.566408	-6.448455	-2.447123
241.H	4.086821	-7.309402	-2.955417
242.H	3.294205	-7.445373	-0.613994
243.H	5.863262	-4.576134	-0.744900
244.H	-0.386926	-2.977444	-0.024795
245.H	-1.666812	-4.956353	-0.318201
246.H	-0.799299	-6.481473	-0.599808
247.P	3.349099	-10.039249	-2.744337
248.O	2.839647	-11.592248	-2.154345
249.O	3.703027	-9.801666	-4.299020
250.O	1.963787	-9.087138	-2.306799
251.C	1.201953	-9.319736	-0.994666
252.C	-0.297587	-9.434359	-1.263001
253.O	-0.914559	-8.081939	-1.509619
254.C	-0.730916	-10.268995	-2.488545
255.O	-2.078688	-10.884784	-2.243572
256.C	-0.773411	-9.246782	-3.647615
257.C	-1.245204	-7.928058	-2.986828
258.N	-0.601204	-6.715958	-3.455961
259.C	0.775219	-6.459153	-3.473642
260.N	1.041224	-5.171705	-3.573711
261.C	-0.202464	-4.531314	-3.600323
262.C	-0.538316	-3.153049	-3.539530
263.O	0.248088	-2.166609	-3.481059
264.N	-1.932323	-2.941807	-3.507578
265.N	6.316899	-2.685377	2.588605
266.C	-1.213405	-6.573357	2.692387
267.C	-1.236918	-5.475809	-3.530580
268.H	1.404510	-8.436353	-0.383295
269.H	1.572827	-10.236199	-0.523900
270.H	-7.383434	-7.895404	0.644094
271.H	-0.752674	-9.812300	-0.339073
272.H	4.822216	4.564440	-3.458569
273.H	-8.359261	-8.320904	-0.820809
274.C	-3.551806	-7.321432	2.006058
275.H	-9.197567	-6.251836	0.248793
276.O	-8.133385	0.948309	-1.216925
277.H	-0.061744	-11.112540	-2.678932
278.C	-2.882648	-3.950090	-3.539616
279.N	-4.178564	-3.589307	-3.591474

280.N	-2.562442	-5.254953	-3.516142
281.H	0.230357	-9.131502	-4.068926
282.O	-1.109592	-9.756720	1.989063
283.H	-7.468408	-3.273321	-0.436442
284.C	7.953325	-3.116278	0.755774
285.N	-2.588484	-6.370235	2.531407
286.H	-4.606458	-5.838403	-0.716704
287.H	-2.325907	-7.776622	-3.046985
288.H	-8.907059	-6.248171	-2.493750
289.C	7.280884	-3.628803	2.050176
290.N	-0.583595	-5.459628	3.017403
291.C	-1.570639	-4.471080	3.064792
292.C	-1.473080	-3.068061	3.265745
293.O	-9.679046	1.071225	2.337650
294.C	-10.386615	2.211190	3.013048
295.C	-9.690852	3.513249	2.620421
296.O	-8.356567	3.644073	3.333301
297.C	-9.360495	3.592687	1.120754
298.O	-9.440875	5.098241	0.786779
299.C	-7.928043	3.079031	1.009347
300.C	-7.241304	3.508924	2.325945
301.N	-6.274820	2.532221	2.796266
302.C	-6.473661	1.153707	2.931722
303.N	-5.350468	0.516409	3.205655
304.C	-4.359973	1.502006	3.243254
305.C	-2.951574	1.400149	3.398412
306.O	-2.259226	0.351125	3.523067
307.N	-2.317588	2.661150	3.371331
308.C	-2.975272	3.872334	3.208347
309.N	-2.241580	5.002441	3.277645
310.N	-4.298878	3.960681	3.003269
311.C	-4.920987	2.768751	3.015693
312.H	-10.341340	2.090419	4.103218
313.H	-11.433030	2.245116	2.676925
314.H	-10.300341	4.368066	2.936450
315.H	-10.081278	3.069140	0.489958
316.H	-7.974587	1.993453	0.949328
317.H	-7.408369	3.435457	0.119831
318.H	-6.727711	4.473076	2.257753
319.H	-7.463839	0.724061	2.824616
320.H	-1.282280	2.644804	3.479138
321.H	-1.203393	5.016298	3.300873
322.H	-2.720150	5.857575	3.014344
323.P	-9.104590	5.539248	-0.893703
324.O	-10.213475	6.849088	-1.177077
325.O	-9.052873	4.282506	-1.903079
326.O	-7.611370	6.427770	-0.834250
327.C	-7.609183	7.687208	0.056032
328.C	-6.212128	8.293333	0.046997
329.O	-5.231591	7.334787	0.685320
330.C	-5.613512	8.616492	-1.338734
331.O	-4.634906	9.767067	-1.002616
332.C	-4.846141	7.346594	-1.707224
333.C	-4.214169	6.944897	-0.358162
334.N	-3.922751	5.541985	-0.220275
335.C	-4.804742	4.466541	-0.289210
336.N	-4.181393	3.309639	-0.178841
337.C	-2.825840	3.623043	-0.046708
338.C	-1.672745	2.805227	0.072621
339.O	-1.617168	1.542235	0.127428
340.N	-0.482585	3.558094	0.122029
341.C	-0.412090	4.946145	0.044092
342.N	0.793040	5.527953	0.022243
343.N	-1.511028	5.719223	-0.009400
344.C	-2.646743	5.016629	-0.072091
345.H	-7.869377	7.375561	1.072751
346.H	-8.344213	8.387339	-0.351998
347.H	-6.239619	9.199426	0.666394
348.H	-6.329891	8.976306	-2.081275

349.H	-5.580792	6.597842	-2.024856
350.H	-4.104284	7.483065	-2.499273
351.H	-3.287149	7.486226	-0.163166
352.H	-5.862832	4.631595	-0.430883
353.H	0.391230	2.989185	0.141040
354.H	1.670262	4.980389	-0.064827
355.H	0.800521	6.519321	-0.246714
356.P	-3.362266	10.201888	-2.148695
357.O	-2.844867	11.719079	-1.477796
358.O	-3.729779	10.051861	-3.711073
359.O	-1.976771	9.223445	-1.775002
360.C	-1.205724	9.376755	-0.456583
361.C	0.292010	9.506548	-0.728578
362.O	0.906459	8.171036	-1.059059
363.C	0.714681	10.411470	-1.907088
364.O	2.064191	11.012944	-1.638559
365.C	0.746286	9.458452	-3.124075
366.C	1.222881	8.103239	-2.545740
367.N	0.573011	6.920569	-3.077779
368.C	-0.803592	6.664184	-3.092191
369.N	-1.070885	5.384327	-3.261558
370.C	0.172304	4.747360	-3.340911
371.C	0.508672	3.367985	-3.363744
372.O	-0.277135	2.379517	-3.351262
373.N	1.902969	3.156289	-3.362674
374.C	2.852785	4.165510	-3.351419
375.N	4.147571	3.809081	-3.446603
376.N	2.533151	5.466683	-3.248902
377.C	1.207533	5.686995	-3.231465
378.H	-1.404530	8.458311	0.102006
379.H	-1.572637	10.263321	0.071234
380.H	0.754963	9.829925	0.212077
381.H	0.043453	11.264165	-2.041646
382.H	-0.261262	9.367905	-3.542284
383.H	1.426221	9.824938	-3.902885
384.H	2.302762	7.955130	-2.625439
385.H	-1.519498	7.459480	-2.934308
386.H	2.201233	2.158074	-3.405599
387.H	4.485895	2.826183	-3.452133
388.H	10.241492	-2.718343	-2.153231
389.H	-10.251574	2.860900	-1.887837
390.H	-2.798336	-10.178115	-2.297398
391.H	-1.460353	-9.567786	-4.440167
392.H	2.784244	10.312669	-1.745302
393.H	-11.175977	6.570797	-1.273731
394.H	-3.524601	12.458060	-1.539513
395.H	6.520993	11.224829	-1.232649
396.H	-10.106744	0.220998	2.635075
397.H	-6.533332	-11.121520	-1.774824
398.H	12.383743	3.588003	-1.852224
399.H	0.303538	10.038403	2.867517
400.H	10.146190	-0.358089	2.529924
401.K	-0.009130	0.061070	-1.827231
402.K	0.014668	-0.051014	1.915745

Table S22 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of **GQ–K⁺–Rb⁺** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

GQ–K⁺–Rb⁺ (Bond Energy: -55749.77 kcal/mol)			
1.C	6.526285	-1.344254	2.822529
2.N	5.419297	-0.726859	3.191570
3.C	4.423611	-1.707639	3.179457
4.C	3.026672	-1.612103	3.416490
5.O	2.355824	-0.575932	3.682304
6.N	2.375866	-2.860917	3.290532
7.C	3.013832	-4.055840	2.983859
8.N	2.269914	-5.181481	2.969438

9.N	4.327473	-4.133523	2.719536
10.C	4.963276	-2.952159	2.817408
11.H	10.366869	-2.353381	3.887837
12.H	11.464130	-2.411976	2.458548
13.H	10.333242	-4.544766	2.558369
14.H	10.102968	-3.071076	0.213808
15.H	7.997334	-2.035581	0.758108
16.H	7.429162	-3.412572	-0.172638
17.H	6.751831	-4.602043	1.888257
18.H	7.516468	-0.913094	2.720652
19.H	1.349701	-2.855366	3.457008
20.H	1.234833	-5.195742	3.040050
21.H	2.729182	-6.012234	2.611232
22.P	9.107180	-5.447787	-1.332040
23.O	10.210093	-6.735041	-1.720492
24.O	9.036383	-4.128434	-2.256680
25.O	7.617048	-6.343921	-1.300339
26.C	7.638189	-7.653755	-0.485463
27.C	-2.799629	-1.687890	-0.098186
28.C	6.243385	-8.264516	-0.498241
29.O	5.273599	-7.345861	0.211901
30.C	5.616475	-8.513558	-1.886388
31.O	4.643846	-9.680469	-1.592429
32.C	4.840330	-7.227665	-2.169597
33.C	4.234637	-6.903285	-0.787895
34.H	-2.741975	4.603283	-3.380256
35.N	3.944500	-5.510220	-0.570280
36.H	-4.479433	4.938689	-3.396285
37.H	-4.974741	1.661300	-0.125042
38.N	-3.551580	-0.498365	-0.018551
39.N	-5.070675	-2.332811	3.093285
40.H	-6.507779	0.800043	-0.348836
41.C	-4.939336	-0.425046	-0.091292
42.H	-6.541190	-5.504856	-2.369870
43.O	-1.536384	-1.633312	-0.048731
44.H	-7.416700	-4.010167	-2.803156
45.H	-9.826996	0.750725	0.015459
46.H	-11.208364	0.131261	-2.298984
47.H	-9.274704	-0.130747	-3.759131
48.H	-9.714052	1.571246	-4.070627
49.H	-7.876734	2.390901	-2.710221
50.H	1.503444	-7.262009	-3.353045
51.C	4.825987	-4.432029	-0.596629
52.N	4.203997	-3.281484	-0.427638
53.O	-0.444016	-2.432274	3.648790
54.C	-3.945664	-3.076597	3.054477
55.C	-2.296785	-10.472804	2.622258
56.N	-2.741050	-2.445288	3.335837
57.H	-12.403504	-3.503183	-1.914385
58.H	-7.377239	-1.418072	-3.141255
59.C	-5.009712	-2.655726	-0.277421
60.H	-2.072633	2.318577	-3.427328
61.H	3.530882	-12.331441	-2.229844
62.H	11.170677	-6.451284	-1.817932
63.N	-4.032371	-4.383792	2.762407
64.C	-2.848120	-5.020419	2.803029
65.N	-5.520744	0.781712	-0.063990
66.O	1.171850	9.624297	2.540205
67.C	2.341122	10.304301	3.193902
68.C	3.624231	9.626302	2.716911
69.O	3.795976	8.270460	3.378366
70.C	3.632052	9.344980	1.205552
71.O	5.119385	9.447342	0.805616
72.C	3.118204	7.913906	1.072461
73.C	3.609627	7.186139	2.344797
74.N	2.652961	6.210193	2.835942
75.C	1.287932	6.419101	3.062020
76.N	0.662055	5.301495	3.381528
77.C	1.642452	4.305566	3.358579

78.C	1.541900	2.902546	3.552835
79.O	0.500655	2.225140	3.779655
80.N	2.792621	2.254516	3.431706
81.C	3.993941	2.900377	3.169639
82.N	5.118661	2.155600	3.152742
83.N	4.077892	4.221770	2.949272
84.C	2.894812	4.855232	3.041452
85.H	2.267630	10.215523	4.285568
86.H	2.361545	11.363297	2.898555
87.H	4.491571	10.229066	3.010736
88.H	3.075670	10.082168	0.623635
89.H	2.030862	7.958673	1.064145
90.H	3.433074	7.424806	0.150663
91.H	4.567649	6.672974	2.215302
92.H	0.859566	7.412543	2.982556
93.H	2.783244	1.223531	3.564779
94.H	5.131771	1.119095	3.196944
95.H	5.957610	2.624568	2.827954
96.P	5.492266	9.154182	-0.898236
97.O	6.790620	10.269285	-1.205384
98.O	4.196648	9.122842	-1.858142
99.O	6.385712	7.661634	-0.903404
100.C	7.675015	7.648651	-0.056125
101.C	8.283428	6.253560	-0.104528
102.O	7.346914	5.260566	0.547459
103.C	8.566295	5.676754	-1.508019
104.O	9.727444	4.695362	-1.220942
105.C	7.287737	4.912038	-1.850014
106.C	6.928892	4.257875	-0.499253
107.N	5.530951	3.961320	-0.325842
108.C	4.453445	4.843722	-0.351536
109.N	3.299352	4.217752	-0.227197
110.C	3.617706	2.860539	-0.130480
111.C	2.802033	1.704798	-0.037693
112.O	1.539474	1.647489	0.024988
113.N	3.554802	0.513209	-0.029063
114.C	4.941988	0.444809	-0.118707
115.N	5.523729	-0.761332	-0.159807
116.N	5.713803	1.544867	-0.163452
117.C	5.010242	2.682203	-0.189890
118.H	7.397428	7.894319	0.974000
119.H	8.359628	8.390728	-0.477344
120.H	9.207738	6.274332	0.487627
121.H	8.902832	6.404893	-2.250002
122.H	6.527868	5.649579	-2.132742
123.H	7.401281	4.183529	-2.657901
124.H	7.477853	3.329241	-0.335102
125.H	4.615691	5.904365	-0.476034
126.H	2.988609	-0.362548	-0.032088
127.H	4.976431	-1.636378	-0.262674
128.H	6.507748	-0.764537	-0.455548
129.P	10.123892	3.435911	-2.394812
130.O	11.658038	2.907045	-1.774324
131.O	9.928771	3.824587	-3.947059
132.O	9.153073	2.047598	-2.011905
133.C	9.358822	1.242663	-0.720988
134.C	9.474566	-0.247408	-1.037405
135.O	8.126037	-0.848892	-1.337046
136.C	10.336393	-0.639815	-2.258274
137.O	10.943432	-1.997161	-2.047185
138.C	9.341117	-0.638902	-3.441197
139.C	8.006890	-1.130439	-2.827536
140.N	6.806717	-0.470379	-3.304094
141.C	6.548027	0.905320	-3.280364
142.N	5.263796	1.173819	-3.412203
143.C	4.627386	-0.068909	-3.504625
144.C	3.248482	-0.407882	-3.508065
145.O	2.259103	0.375385	-3.461511
146.N	3.039525	-1.802503	-3.531937

147.C	4.050308	-2.750268	-3.561874
148.N	3.693500	-4.044108	-3.672477
149.N	5.352819	-2.429849	-3.484041
150.C	5.571094	-1.104420	-3.441632
151.H	8.464420	1.428794	-0.120446
152.H	10.266787	1.595305	-0.220803
153.H	9.830537	-0.736900	-0.122020
154.H	11.185443	0.033488	-2.405072
155.H	9.236597	0.379179	-3.829601
156.H	9.679014	-1.298219	-4.250053
157.H	7.856469	-2.208228	-2.927827
158.H	7.346123	1.618700	-3.125238
159.H	2.041470	-2.102497	-3.560378
160.H	2.711887	-4.384749	-3.658021
161.H	4.449266	-4.717337	-3.710552
162.H	-4.846892	-4.353453	-3.656831
163.H	-2.227167	-1.949268	-3.539534
164.P	-10.144754	-3.290675	-2.496632
165.O	-11.681535	-2.805990	-1.845965
166.O	-9.953105	-3.603139	-4.066377
167.O	-9.185238	-1.911552	-2.053656
168.H	-2.209688	-10.454348	3.716437
169.H	-2.322251	-11.510676	2.259958
170.H	-4.449526	-10.383501	2.474838
171.H	-2.009893	-8.003054	0.637042
172.H	-3.421666	-7.412734	-0.225512
173.H	-4.531170	-6.788403	1.895344
174.H	-0.812623	-7.567537	2.568476
175.C	-9.373597	-1.189126	-0.712412
176.H	-0.295344	-10.194436	2.308062
177.H	-2.985145	0.376441	0.019240
178.H	-2.730202	-1.423580	3.527171
179.H	-5.082722	-1.299797	3.188700
180.H	-5.913810	-2.784789	2.755449
181.P	-5.498784	-9.069855	-1.348902
182.O	-6.794866	-10.172602	-1.708953
183.O	-4.213361	-8.977795	-2.318508
184.H	-4.511966	-2.617744	-3.572694
185.O	-6.397195	-7.583620	-1.263349
186.C	-7.679364	-7.620695	-0.406379
187.C	-8.286827	-6.224964	-0.369958
188.O	-7.344503	-5.272795	0.333092
189.C	-8.576342	-5.567401	-1.735997
190.O	-9.733270	-4.601824	-1.386264
191.C	-7.299024	-4.784990	-2.040175
192.O	-5.107350	-9.462996	0.330763
193.H	-10.279994	-1.566890	-0.227666
194.N	-5.712254	-1.521085	-0.186120
195.C	-9.483801	0.318481	-0.932857
196.C	-9.371558	0.861730	-3.307430
197.C	-3.096906	-7.957051	0.661344
198.C	-6.932095	-4.211115	-0.655542
199.N	-5.532741	-3.925808	-0.473986
200.C	-4.456309	-4.805827	-0.558012
201.C	-10.355683	0.791321	-2.117425
202.H	-3.069488	-10.094854	0.080804
203.C	-8.029820	1.309202	-2.676965
204.N	-6.836572	0.677290	-3.206406
205.C	-6.579658	-0.697720	-3.264097
206.N	-3.300485	-4.187674	-0.412864
207.N	-5.297296	-0.959188	-3.425470
208.C	-4.660279	0.286280	-3.454744
209.C	-3.281034	0.624346	-3.457596
210.O	-2.291880	-0.160462	-3.467649
211.N	-3.070714	2.018005	-3.406341
212.C	-3.616748	-2.837284	-0.241648
213.C	-3.585053	-9.765241	2.205838
214.O	-3.743785	-8.451481	2.950657
215.O	-10.955733	2.134018	-1.813467

216.C	-3.613747	-9.392249	0.714625
217.C	-4.080620	2.966409	-3.368723
218.O	9.714240	-1.214052	2.192957
219.N	-3.723863	4.264300	-3.412093
220.C	10.416468	-2.399340	2.792131
221.C	9.721048	-3.670493	2.307909
222.O	8.389508	-3.858719	3.012985
223.N	-5.382394	2.642741	-3.292552
224.C	9.385738	-3.640738	0.807817
225.C	-5.601823	1.317141	-3.322520
226.H	-8.475770	-1.416868	-0.131681
227.O	9.470544	-5.118046	0.367516
228.C	2.850044	-3.602770	-0.299887
229.C	1.697429	-2.790343	-0.155894
230.O	1.641662	-1.529519	-0.063840
231.N	0.506612	-3.543957	-0.130585
232.C	0.435479	-4.928720	-0.249955
233.N	-0.771349	-5.509963	-0.269037
234.N	1.533739	-5.698475	-0.345072
235.C	2.669916	-4.993602	-0.386763
236.H	7.920122	-7.400462	0.541605
237.H	8.366222	-8.325433	-0.949773
238.H	6.286449	-9.202812	0.070188
239.H	6.317235	-8.832172	-2.661871
240.H	5.567120	-6.460128	-2.459162
241.H	4.083338	-7.321779	-2.953477
242.H	3.312370	-7.456909	-0.604430
243.H	5.882611	-4.591239	-0.754421
244.H	-0.368819	-2.978599	-0.092290
245.H	-1.649607	-4.961416	-0.327949
246.H	-0.784408	-6.487057	-0.586575
247.P	3.352587	-10.052045	-2.739615
248.O	2.843325	-11.602398	-2.142928
249.O	3.699178	-9.818906	-4.296618
250.O	1.971940	-9.095258	-2.297148
251.C	1.209974	-9.328568	-0.985206
252.C	-0.289737	-9.438934	-1.254362
253.O	-0.901546	-8.084250	-1.501759
254.C	-0.723477	-10.272426	-2.480753
255.O	-2.072448	-10.886143	-2.237385
256.C	-0.763111	-9.249718	-3.639369
257.C	-1.233870	-7.930677	-2.978500
258.N	-0.590248	-6.719078	-3.449049
259.C	0.785700	-6.460694	-3.465764
260.N	1.050308	-5.173608	-3.576059
261.C	-0.194411	-4.535507	-3.611439
262.C	-0.532508	-3.156954	-3.570852
263.O	0.252274	-2.168645	-3.526985
264.N	-1.926967	-2.947649	-3.542759
265.N	6.310818	-2.704250	2.573005
266.C	-1.240315	-6.580799	2.710359
267.C	-1.227785	-5.480706	-3.535683
268.H	1.415085	-8.446799	-0.372357
269.H	1.578765	-10.246725	-0.516146
270.H	-7.393528	-7.924674	0.605736
271.H	-0.747796	-9.815632	-0.331273
272.H	4.814825	4.574968	-3.460084
273.H	-8.367298	-8.337766	-0.863949
274.C	-3.571318	-7.307155	1.981300
275.H	-9.207572	-6.278742	0.225652
276.O	-8.135191	0.932363	-1.206968
277.H	-0.055272	-11.116867	-2.670615
278.C	-2.875835	-3.957607	-3.563194
279.N	-4.172474	-3.598656	-3.620748
280.N	-2.553780	-5.261561	-3.526897
281.H	0.241350	-9.135335	-4.059238
282.O	-1.134519	-9.752988	1.999410
283.H	-7.479292	-3.293375	-0.433881
284.C	7.951368	-3.122743	0.739248

285.N	-2.608688	-6.361156	2.516822
286.H	-4.621015	-5.858436	-0.735975
287.H	-2.314557	-7.779049	-3.038361
288.H	-8.918187	-6.250998	-2.516885
289.C	7.269159	-3.647069	2.023844
290.N	-0.610353	-5.482326	3.083620
291.C	-1.591487	-4.488117	3.132667
292.C	-1.488426	-3.097579	3.401944
293.O	-9.672680	1.092643	2.349471
294.C	-10.368450	2.239400	3.025779
295.C	-9.676456	3.537641	2.614077
296.O	-8.337429	3.681191	3.315434
297.C	-9.356155	3.601160	1.111845
298.O	-9.439025	5.103709	0.766323
299.C	-7.924439	3.085146	0.996319
300.C	-7.227944	3.529091	2.303106
301.N	-6.265292	2.554214	2.784351
302.C	-6.479962	1.182506	2.958057
303.N	-5.370400	0.544638	3.282181
304.C	-4.374004	1.524254	3.317590
305.C	-2.975653	1.415837	3.540304
306.O	-2.303480	0.366859	3.746123
307.N	-2.324772	2.669374	3.477177
308.C	-2.964112	3.879626	3.241560
309.N	-2.219066	5.003781	3.281265
310.N	-4.279963	3.972211	2.993920
311.C	-4.915670	2.787367	3.030800
312.H	-10.309263	2.126659	4.116129
313.H	-11.419118	2.272897	2.703080
314.H	-10.285139	4.394960	2.924710
315.H	-10.080982	3.071933	0.490415
316.H	-7.973204	1.998981	0.948779
317.H	-7.411275	3.430150	0.098659
318.H	-6.710837	4.490125	2.220470
319.H	-7.471336	0.758250	2.840121
320.H	-1.297351	2.654829	3.634637
321.H	-1.183426	5.014131	3.343578
322.H	-2.680800	5.853418	2.974197
323.P	-9.110448	5.536770	-0.916809
324.O	-10.228691	6.837201	-1.206252
325.O	-9.051227	4.274721	-1.919266
326.O	-7.624035	6.436893	-0.862783
327.C	-7.631082	7.697274	0.026513
328.C	-6.233875	8.302811	0.031047
329.O	-5.259670	7.341844	0.675920
330.C	-5.623197	8.628517	-1.348750
331.O	-4.647199	9.778057	-1.002242
332.C	-4.852875	7.359242	-1.712883
333.C	-4.232967	6.954901	-0.358875
334.N	-3.943316	5.551022	-0.223342
335.C	-4.826376	4.476709	-0.304304
336.N	-4.204926	3.317671	-0.205551
337.C	-2.849508	3.629773	-0.069626
338.C	-1.696586	2.809526	0.018786
339.O	-1.641291	1.545506	0.038741
340.N	-0.504532	3.559619	0.077214
341.C	-0.432725	4.948754	0.034646
342.N	0.774496	5.529572	0.035298
343.N	-1.530843	5.723507	-0.005969
344.C	-2.668170	5.023286	-0.078317
345.H	-7.901645	7.386781	1.040866
346.H	-8.362026	8.396622	-0.390064
347.H	-6.265829	9.207520	0.652097
348.H	-6.333131	8.989749	-2.096759
349.H	-5.584987	6.611158	-2.037973
350.H	-4.104336	7.496621	-2.498434
351.H	-3.307546	7.495573	-0.154349
352.H	-5.883859	4.645474	-0.445655
353.H	0.370630	2.992537	0.073640

354.H	1.650982	4.984905	-0.069045
355.H	0.784320	6.523063	-0.226632
356.P	-3.366407	10.214469	-2.138430
357.O	-2.848990	11.727375	-1.458304
358.O	-3.724673	10.071503	-3.703578
359.O	-1.986192	9.229953	-1.760309
360.C	-1.214844	9.383309	-0.442010
361.C	0.283001	9.509187	-0.715176
362.O	0.892656	8.171510	-1.046234
363.C	0.705861	10.412796	-1.894838
364.O	2.056612	11.012259	-1.628291
365.C	0.734920	9.459073	-3.111205
366.C	1.210557	8.103668	-2.532425
367.N	0.561049	6.921551	-3.065718
368.C	-0.815011	6.663558	-3.079745
369.N	-1.080949	5.384877	-3.261117
370.C	0.163204	4.750829	-3.349721
371.C	0.501681	3.372441	-3.395273
372.O	-0.282571	2.382821	-3.399905
373.N	1.896409	3.163038	-3.397495
374.C	2.844849	4.173298	-3.372431
375.N	4.140460	3.819290	-3.471755
376.N	2.523357	5.472669	-3.255959
377.C	1.197364	5.690763	-3.232817
378.H	-1.416179	8.466118	0.117728
379.H	-1.579718	10.271381	0.084635
380.H	0.748943	9.831756	0.224405
381.H	0.035550	11.266292	-2.028922
382.H	-0.273093	9.369135	-3.528384
383.H	1.414349	9.824117	-3.891147
384.H	2.290425	7.955353	-2.612040
385.H	-1.531266	7.456701	-2.912440
386.H	2.196432	2.165936	-3.449543
387.H	4.480530	2.837180	-3.470880
388.H	10.239078	-2.712760	-2.156102
389.H	-10.251920	2.854313	-1.889319
390.H	-2.791672	-10.179980	-2.301246
391.H	-1.449355	-9.569244	-4.433121
392.H	2.776116	10.313300	-1.746374
393.H	-11.190681	6.553393	-1.291351
394.H	-3.526672	12.468218	-1.520014
395.H	6.507839	11.230980	-1.294019
396.H	-10.102649	0.246049	2.654006
397.H	-6.513749	-11.134179	-1.805978
398.H	12.394076	3.589700	-1.838052
399.H	0.335977	10.043117	2.887070
400.H	10.146243	-0.387257	2.545381
401.K	-0.009702	0.061925	-1.881812
402.Rb	0.012767	-0.049735	1.974946

Table S23 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of the **guanine monomer (G)** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

Guanine monomer (G) (Bond Energy: -2468.79 kcal/mol)			
1.N	-3.071552	2.085759	0.000640
2.N	0.477214	3.879839	-0.032898
3.C	0.473526	2.498689	-0.040975
4.N	-0.645397	1.777361	-0.027682
5.C	-1.769970	2.538346	-0.014035
6.C	-1.871257	3.940977	-0.004181
7.C	-0.671490	4.718373	-0.014319
8.C	-3.895271	3.200238	0.017643
9.N	-3.211759	4.336219	0.015463
10.O	-0.534304	5.962545	-0.009013
11.N	1.688530	1.872463	-0.124318
12.H	-4.974367	3.108080	0.031719
13.H	1.676364	0.884207	0.114750

14.H	2.507043	2.375389	0.207893
15.H	1.370918	4.370357	-0.056547
16.H	-3.371070	1.114161	-0.001685

Table S24 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of the **guanosine dimer (GG)** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

Guanosine dimer (GG) (Bond Energy: -9170.05 kcal/mol)			
1.C	-9.045306	-5.036249	0.168612
2.O	-3.088383	-7.857953	2.660591
3.O	-10.171868	-4.090109	0.495332
4.C	-8.193722	-4.511311	-1.007224
5.O	-5.461202	-9.117984	1.324762
6.H	-6.476771	-6.060367	2.307856
7.C	-3.981876	-9.203113	0.864041
8.C	-3.514860	-7.875937	0.265344
9.H	-0.118693	-9.640978	1.143601
10.C	-7.155067	-3.546583	-0.372077
11.O	-1.068995	-9.357413	1.031349
12.H	-3.879951	-10.077371	0.216031
13.H	-8.194090	-10.147832	1.102658
14.O	-6.887369	-6.876887	0.383201
15.C	-7.364450	-6.270250	1.705194
16.C	-3.443047	-6.952767	1.498122
17.H	-7.421717	-2.492066	-0.479025
18.H	-1.356733	-9.821809	3.100569
19.H	-2.003443	-11.049144	1.951748
20.H	-3.855787	-9.805964	2.956775
21.H	-2.516350	-8.037376	-0.154919
22.H	-4.166830	-7.479683	-0.516278
23.P	-6.699246	-8.591124	0.190966
24.H	-4.406103	-6.489152	1.720875
25.C	-8.115710	-4.979191	1.394204
26.H	-7.702078	-5.355360	-1.498229
27.H	-8.809495	-3.987180	-1.748731
28.H	-8.029701	-6.986709	2.198475
29.H	-9.443893	-6.040866	-0.014244
30.C	-3.236155	-9.297377	2.208079
31.O	-7.180842	-3.835020	1.113854
32.H	-8.681960	-4.691620	2.289272
33.C	-1.868604	-9.973983	2.141041
34.H	-10.782304	-4.053413	-0.296662
35.O	-8.130684	-9.148071	1.012240
36.O	-6.448513	-8.936645	-1.364187
37.H	-3.165998	1.238761	-0.597984
38.N	-2.761000	-1.162309	-1.341745
39.N	-5.256452	-2.192426	2.482168
40.H	-4.838629	1.059928	-0.226130
41.C	-3.965604	-0.635120	-0.919581
42.N	-5.055666	-1.378856	-0.730996
43.O	-1.378196	-2.884606	-2.035248
44.C	-2.507870	-2.533095	-1.640696
45.H	-0.625146	-6.860046	0.890990
46.N	-2.480695	-5.881243	1.419060
47.H	-5.651393	-5.845078	-1.170398
48.C	-1.635830	-2.421528	1.644587
49.C	-3.677180	-3.325143	-1.414634
50.N	-5.800610	-3.709173	-0.876136
51.C	-5.140300	-4.895519	-1.213568
52.C	-1.120133	-5.919190	1.101908
53.O	-0.714254	-1.586690	1.526761
54.C	-4.069489	-2.778647	2.139462
55.N	-3.878861	-4.701225	-1.548223
56.N	-2.954524	-1.975730	1.972837
57.H	-1.966289	-0.537704	-1.477415
58.C	-4.856758	-2.692867	-0.991994
59.H	-6.066222	-2.758302	2.184635

60.N	-0.567043	-4.717165	1.131328
61.C	-1.604608	-3.842427	1.480556
62.N	-4.018721	-4.100364	2.002158
63.C	-2.794767	-4.556255	1.672725
64.N	-4.025021	0.713257	-0.725331
65.H	-3.042190	-0.970598	2.120084
66.H	-5.351005	-1.201482	2.273592

Table S25 Cartesian coordinates (in Å) and ADF total bonding energies (in kcal/mol) of the **guanosine trimer (GGG)** at the ZORA-BLYP-D3(BJ)/TZP/DZ level of theory with COSMO to simulate water.

Guanosine trimer (GGG) (Bond Energy: -13893.19 kcal/mol)			
1 C	-0.194440000000	-3.012456000000	-3.598720000000
2 C	6.130067000000	-1.445246000000	2.329099000000
3 N	5.012847000000	-0.878855000000	2.784049000000
4 H	9.653290000000	-2.522316000000	4.031250000000
5 H	10.983909000000	-2.466298000000	2.817262000000
6 H	9.926049000000	-4.624350000000	2.620769000000
7 H	10.081148000000	-3.093087000000	0.305704000000
8 H	7.897346000000	-2.090552000000	0.457278000000
9 H	7.520276000000	-3.492511000000	-0.550151000000
10 H	6.469456000000	-4.669179000000	1.324866000000
11 H	-4.565844000000	-3.985860000000	-2.990789000000
12 H	-1.857927000000	-1.777984000000	-3.511257000000
13 H	7.101587000000	-0.973254000000	2.230868000000
14 H	1.159712000000	-3.264371000000	3.416193000000
15 H	-4.098231000000	-2.323986000000	-3.249278000000
16 H	1.183982000000	-5.572592000000	3.045592000000
17 C	4.075017000000	-1.891511000000	2.796890000000
18 H	2.608675000000	-6.317344000000	2.372305000000
19 P	9.228940000000	-5.633485000000	-1.329393000000
20 O	9.267122000000	-1.297045000000	2.315678000000
21 C	9.893808000000	-2.497671000000	2.960076000000
22 O	10.343215000000	-6.966982000000	-1.476700000000
23 C	9.342701000000	-3.755242000000	2.295175000000
24 O	7.912281000000	-4.026101000000	2.727114000000
25 C	9.282468000000	-3.685341000000	0.759223000000
26 O	9.486164000000	-5.155048000000	0.347892000000
27 C	2.882008000000	-3.472408000000	-0.614225000000
28 C	1.745854000000	-2.669470000000	-0.254782000000
29 O	1.670377000000	-1.439987000000	-0.116090000000
30 O	9.193848000000	-4.459699000000	-2.433661000000
31 N	0.592234000000	-3.489403000000	-0.031092000000
32 C	0.539867000000	-4.867172000000	-0.135338000000
33 N	-0.632948000000	-5.493358000000	0.040051000000
34 N	1.632016000000	-5.607169000000	-0.410673000000
35 C	2.726663000000	-4.872270000000	-0.637766000000
36 H	7.777609000000	-7.221651000000	0.735393000000
37 H	8.328539000000	-8.412460000000	-0.511731000000
38 H	6.080238000000	-9.034514000000	0.304309000000
39 H	6.495335000000	-8.931853000000	-2.440758000000
40 H	5.794504000000	-6.561857000000	-2.590413000000
41 O	7.726707000000	-6.506666000000	-1.285992000000
42 H	4.344198000000	-7.430355000000	-3.145116000000
43 H	3.341731000000	-7.308773000000	-0.878255000000
44 H	5.836232000000	-4.399133000000	-1.471741000000
45 H	-0.259398000000	-2.977110000000	0.199936000000
46 H	-1.489585000000	-4.968756000000	0.181174000000
47 H	-0.696935000000	-6.483253000000	-0.246092000000
48 P	3.406159000000	-10.023297000000	-2.640607000000
49 O	2.826003000000	-11.538717000000	-2.025037000000
50 O	3.711268000000	-9.822876000000	-4.210734000000
51 O	2.097401000000	-8.987203000000	-2.151525000000
52 C	7.597885000000	-7.636131000000	-0.261892000000
53 C	1.364351000000	-9.200281000000	-0.821096000000
54 C	-0.131248000000	-9.361216000000	-1.081149000000
55 O	-0.812034000000	-8.020892000000	-1.257993000000

56 C	-0.500685000000	-10.149064000000	-2.357904000000
57 O	-1.775748000000	-10.916979000000	-2.160065000000
58 C	-0.633601000000	-9.072680000000	-3.460561000000
59 C	-1.087458000000	-7.779914000000	-2.732496000000
60 N	-0.398552000000	-6.566327000000	-3.145038000000
61 C	0.971839000000	-6.374974000000	-3.321939000000
62 N	1.286792000000	-5.103772000000	-3.541145000000
63 C	0.085119000000	-4.418736000000	-3.490891000000
64 O	0.598786000000	-2.073075000000	-3.783445000000
65 N	-1.585135000000	-2.758508000000	-3.440376000000
66 N	5.961817000000	-2.792084000000	2.028211000000
67 C	-0.986979000000	-5.307148000000	-3.241387000000
68 H	1.554594000000	-8.297393000000	-0.236476000000
69 H	1.763441000000	-10.092702000000	-0.328900000000
70 C	6.178249000000	-8.168562000000	-0.362515000000
71 H	-0.588763000000	-9.809855000000	-0.191200000000
72 H	0.235065000000	-10.919483000000	-2.598878000000
73 C	-2.562728000000	-3.709171000000	-3.224316000000
74 N	-3.834900000000	-3.292187000000	-3.106226000000
75 N	-2.289619000000	-5.021540000000	-3.104328000000
76 O	5.207646000000	-7.106889000000	0.114974000000
77 H	0.335195000000	-8.925652000000	-3.946576000000
78 C	7.870231000000	-3.184353000000	0.437138000000
79 H	-2.159416000000	-7.585590000000	-2.815229000000
80 C	6.980127000000	-3.735148000000	1.579926000000
81 C	5.713027000000	-8.536542000000	-1.788806000000
82 C	2.700323000000	-1.887393000000	3.224098000000
83 O	4.710483000000	-9.683728000000	-1.511141000000
84 C	5.013406000000	-7.271278000000	-2.293866000000
85 C	4.281658000000	-6.779633000000	-1.032683000000
86 N	3.971320000000	-5.371443000000	-0.991440000000
87 H	-2.514008000000	-10.272381000000	-1.954901000000
88 H	-1.364795000000	-9.378543000000	-4.218340000000
89 H	9.593102000000	-0.483592000000	2.793622000000
90 O	2.022892000000	-0.942681000000	3.659403000000
91 H	1.661290000000	-7.204865000000	-3.249144000000
92 N	2.125580000000	-3.185251000000	3.096884000000
93 C	4.804847000000	-4.274314000000	-1.171631000000
94 N	4.183088000000	-3.121345000000	-0.948779000000
95 C	2.785588000000	-4.318085000000	2.671464000000
96 H	3.414205000000	-12.328946000000	-2.226617000000
97 H	11.309975000000	-6.693623000000	-1.534657000000
98 N	2.103986000000	-5.475877000000	2.630497000000
99 N	4.066838000000	-4.310015000000	2.258987000000
100 C	4.645468000000	-3.106773000000	2.348640000000

Table S26 Cartesian coordinates (in Å) and ADF total bonding energy (in kcal/mol) of **G_4–K^+–G_4–K^+–G_4–[ ]–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–K^+–G_4–K^+–G_4–[ ]–G_4 (Bond Energy: -39762.24 kcal/mol)			
1.C	-5.919979	-3.012700	3.344437
2.N	-4.610314	-2.830648	3.333388
3.C	-4.433186	-1.447340	3.335686
4.C	-3.246245	-0.669679	3.293782
5.O	-2.059609	-1.083526	3.232481
6.N	-3.515708	0.716328	3.306088
7.C	-4.785566	1.274396	3.321879
8.N	-4.876157	2.616895	3.336849
9.N	-5.909084	0.536731	3.320686
10.C	-5.676088	-0.790236	3.340471
11.C	4.190578	-3.846346	-0.073947
12.H	0.331830	-7.758648	-3.223771
13.N	0.606388	-6.780124	-3.240579
14.H	4.718897	6.168798	0.072672
15.N	3.880976	5.593753	0.062976
16.C	2.570616	6.052505	0.078421
17.C	1.904819	-6.293246	-3.247152
18.H	-6.430731	-3.966641	3.348985
19.H	-2.675321	1.333944	3.312549

20.H	-4.063927	3.264112	3.368664
21.H	-5.809891	3.007164	3.375107
22.N	1.940993	-4.970410	-3.286676
23.H	7.748271	0.433558	-3.211217
24.N	6.769771	0.708649	-3.217783
25.C	6.283223	2.006864	-3.187087
26.N	1.697414	5.060583	0.061529
27.C	2.078147	2.532901	0.006924
28.N	4.960285	2.044397	-3.222241
29.C	4.560303	0.708712	-3.270719
30.C	3.263971	0.130365	-3.304626
31.O	2.151379	0.727540	-3.310612
32.N	3.306896	-1.278675	-3.328281
33.H	-6.179170	4.738584	0.185060
34.H	3.437553	-3.875001	-3.338246
35.N	-5.604356	3.900898	0.157401
36.H	5.194579	-3.911174	-3.320861
37.H	5.246074	0.090267	-0.020571
38.N	3.183604	1.661657	-0.013661
39.N	2.666879	4.856694	3.268046
40.H	6.417828	1.419132	0.010380
41.C	4.512176	2.068508	-0.004920
42.C	2.464195	3.896018	0.039247
43.O	0.903733	2.062922	-0.009898
44.H	7.650391	1.625349	3.224445
45.N	6.640647	1.736007	3.255287
46.C	5.947500	2.939457	3.301118
47.N	4.638018	2.757113	3.321264
48.C	4.470259	-2.033326	-3.359288
49.C	4.460826	1.374017	3.291258
50.H	-2.876317	7.042715	-2.998975
51.C	-6.063283	2.590575	0.146621
52.N	-5.071615	1.717773	0.107888
53.O	-1.032956	2.037400	3.274060
54.C	1.324411	4.765341	3.291338
55.N	4.342225	-3.375703	-3.447651
56.N	0.767088	3.495029	3.296280
57.C	3.272961	0.597240	3.255382
58.H	6.942009	2.864261	-3.138034
59.C	3.836155	4.211653	0.038803
60.H	2.380110	-1.754074	-3.346444
61.O	2.085269	1.012141	3.235278
62.N	3.542515	-0.788280	3.218159
63.N	0.586073	5.888201	3.304602
64.C	-0.739673	5.654437	3.361455
65.N	5.453527	1.110358	-0.012115
66.N	5.696213	-1.488238	-3.334537
67.C	4.812267	-1.345873	3.183654
68.C	5.681066	-0.140590	-3.275048
69.N	4.902860	-2.688211	3.151223
70.N	5.935409	-0.607839	3.177126
71.C	-3.907001	2.484880	0.097000
72.C	-2.544151	2.099499	0.051532
73.H	1.674170	-7.674105	3.179114
74.N	1.785683	-6.664271	3.203867
75.C	2.990050	-5.971166	3.216884
76.N	2.808285	-4.661578	3.236653
77.C	1.425014	-4.484278	3.241161
78.C	0.647917	-3.296393	3.222920
79.O	1.062610	-2.108884	3.190356
80.N	-0.738110	-3.565413	3.221792
81.C	-1.296643	-4.835153	3.207073
82.N	-2.639279	-4.925397	3.213685
83.N	-0.559387	-5.958623	3.184259
84.C	0.767580	-5.726693	3.214687
85.O	-2.074573	0.925615	0.008701
86.N	-1.672667	3.204982	0.050271
87.C	-2.079237	4.533164	0.088411
88.N	-1.120856	5.474309	0.097277
89.N	-3.371396	4.899236	0.115142
90.C	-4.222376	3.856560	0.126308
91.C	5.703265	0.717803	3.243544
92.H	3.943926	-6.481990	3.211466
93.H	-1.355756	-2.725211	3.242319
94.H	-3.286541	-4.113961	3.261877
95.H	-3.029972	-5.859601	3.230467

96.C	0.604401	-4.570755	-3.299172
97.C	0.024975	-3.274571	-3.318585
98.O	0.621470	-2.161737	-3.340657
99.H	7.087474	-2.343490	-0.077143
100.H	0.625715	-2.954910	-0.050388
101.H	0.069373	-5.257197	-0.032130
102.H	-7.118762	2.353212	0.166603
103.H	-0.658459	2.965352	0.029812
104.H	-0.100796	5.266564	0.090818
105.H	-1.429263	6.437736	0.146728
106.H	-4.751206	-6.159763	0.015459
107.N	-3.913277	-5.584735	0.006895
108.C	-2.602925	-6.043575	-0.009166
109.N	-1.729837	-5.051448	-0.017793
110.C	-2.496702	-3.886731	-0.002388
111.C	-2.111092	-2.523130	-0.011873
112.O	-0.937124	-2.052616	-0.039410
113.N	-3.216580	-1.651839	0.004804
114.C	-4.544859	-2.058981	0.029183
115.N	-5.485846	-1.100974	0.062245
116.N	-4.911128	-3.351316	0.019761
117.C	-3.868549	-4.202425	0.012445
118.H	1.398649	-6.428703	-0.042965
119.H	6.458304	3.893205	3.317929
120.H	2.702458	-1.406569	3.222755
121.H	4.091953	-3.336749	3.190717
122.H	5.837294	-3.078676	3.159115
123.N	-1.384175	-3.317933	-3.304108
124.C	-2.139040	-4.481594	-3.313268
125.H	-2.365845	-7.099314	-0.015698
126.H	-2.976920	-0.637505	0.011044
127.H	-5.277935	-0.081245	0.085755
128.H	-6.449505	-1.410285	0.100217
129.N	-3.483180	-4.354248	-3.365839
130.N	-1.593103	-5.707405	-3.300397
131.C	-0.244380	-5.691742	-3.277601
132.H	-0.445178	7.849518	-3.040968
133.N	-0.720436	6.871527	-3.071346
134.C	-2.018822	6.384817	-3.057671
135.N	-2.056361	5.062929	-3.121554
136.C	-0.720520	4.663697	-3.172132
137.C	-0.142069	3.368217	-3.228648
138.O	-0.739150	2.255963	-3.259516
139.H	-7.860546	-0.345197	-3.048661
140.N	-6.882630	-0.619504	-3.088381
141.C	-6.395955	-1.917778	-3.112135
142.N	-5.074278	-1.953497	-3.180728
143.C	-4.675053	-0.616786	-3.195668
144.C	-3.379671	-0.036981	-3.240130
145.O	-2.267431	-0.632998	-3.289029
146.N	-3.422975	1.372075	-3.217628
147.C	-4.586621	2.126750	-3.196681
148.N	-4.460751	3.471014	-3.242771
149.N	-5.811852	1.580428	-3.159677
150.C	-5.795424	0.231668	-3.145003
151.N	1.267074	3.411495	-3.243726
152.N	-6.613456	-1.808506	3.349696
153.C	-2.961478	5.896910	3.422848
154.C	0.128929	5.784127	-3.147824
155.K	0.001165	-0.016443	1.806475
156.K	-0.039713	0.025703	-1.774436
157.H	2.763427	-6.951678	-3.219725
158.H	-7.053629	-2.776614	-3.074777
159.H	-2.496655	1.848249	-3.241265
160.H	-3.553180	3.968500	-3.150918
161.H	-5.310182	4.002361	-3.083855
162.H	3.899735	5.298303	-3.182099
163.H	1.742559	2.485248	-3.278567
164.H	-1.860116	-2.391213	-3.309437
165.H	-4.015145	-5.206622	-3.225449
166.H	-3.980292	-3.449099	-3.250445
167.H	-1.647319	7.601289	3.384679
168.H	6.147947	-4.728787	-0.098793
169.N	5.572853	-3.890963	-0.084940
170.C	6.031742	-2.580641	-0.072124
171.C	2.022004	4.575044	-3.246054

172.N	3.364798	4.448707	-3.327974
173.N	1.476861	5.800362	-3.198779
174.H	-3.915364	6.407038	3.450040
175.N	5.039638	-1.707580	-0.057626
176.C	3.874890	-2.474510	-0.056560
177.H	2.943756	0.647408	-0.029038
178.H	1.385173	2.654933	3.289423
179.H	3.314641	4.044843	3.295075
180.H	3.057390	5.790621	3.298400
181.C	2.511243	-2.088715	-0.054609
182.O	2.040626	-0.914447	-0.055173
183.N	-1.758163	6.591158	3.392616
184.H	3.863860	3.541785	-3.238491
185.H	2.333526	7.108025	0.099468
186.N	1.640065	-3.194378	-0.060606
187.C	2.047191	-4.522837	-0.067699
188.H	-7.623537	-1.696775	3.349794
189.N	-2.778826	4.587357	3.413692
190.C	-1.395744	4.411107	3.380226
191.C	-0.618564	3.224496	3.321457
192.N	1.089263	-5.464396	-0.054222
193.N	3.339471	-4.888840	-0.087484
194.N	4.878534	3.360774	0.010316
195.C	-6.331591	1.677509	6.561981
196.N	-5.233453	0.937926	6.559677
197.C	-4.177730	1.849833	6.574424
198.C	-2.769481	1.638129	6.551871
199.O	-2.153818	0.542727	6.543386
200.N	-2.052245	2.856557	6.543153
201.C	-2.629362	4.113622	6.605186
202.N	-1.803763	5.181609	6.684624
203.N	-3.957510	4.313048	6.624292
204.C	-4.667883	3.165530	6.594397
205.H	-7.348443	1.307043	6.545466
206.H	-1.013283	2.757377	6.517061
207.H	-0.773831	5.124190	6.562681
208.H	-2.241994	6.088548	6.564933
209.N	5.313169	1.846984	6.575176
210.H	6.891637	-3.878663	6.315061
211.N	6.215231	-3.120999	6.351401
212.C	6.502865	-1.764638	6.372022
213.N	5.406062	-1.025556	6.431297
214.C	4.350254	-1.937550	6.443306
215.O	0.672544	2.198146	6.552645
216.C	4.243570	2.672345	6.514896
217.N	2.985107	2.095423	6.492092
218.C	2.942225	-1.725425	6.467854
219.O	2.327659	-0.630348	6.514617
220.N	2.223473	-2.942405	6.434780
221.N	4.443864	4.000482	6.515173
222.C	3.296238	4.711276	6.510697
223.C	2.800951	-4.200969	6.438269
224.N	1.977417	-5.271238	6.510320
225.N	4.128840	-4.400747	6.409712
226.H	-3.751811	-6.852481	6.428060
227.N	-2.994040	-6.175247	6.435451
228.C	-1.637493	-6.461640	6.412484
229.N	-0.897958	-5.363840	6.439702
230.C	-1.810118	-4.308721	6.474953
231.C	-1.598311	-2.900450	6.486410
232.O	-0.502704	-2.285249	6.496812
233.N	-2.816572	-2.182729	6.488333
234.C	-4.073958	-2.761127	6.533369
235.N	-5.142137	-1.937689	6.630342
236.N	-4.273345	-4.089370	6.519642
237.C	-3.125800	-4.799100	6.477445
238.C	4.839353	-3.252970	6.399304
239.H	-1.266920	-7.477798	6.373243
240.H	-2.716835	-1.143449	6.482444
241.H	-5.083562	-0.904984	6.535349
242.H	-6.048596	-2.372290	6.494687
243.H	7.519168	-1.393822	6.338843
244.H	1.184268	-2.841587	6.430442
245.H	0.944584	-5.209438	6.418545
246.H	2.410596	-6.172512	6.339572
247.N	-6.044635	3.033935	6.584562

248.C	1.808140	6.375267	6.503527
249.C	1.767984	2.813490	6.528315
250.H	3.922660	6.764684	6.471268
251.H	1.437596	7.392090	6.487166
252.H	2.884523	1.056425	6.471374
253.H	5.252058	0.816506	6.459349
254.H	6.215958	2.283801	6.422828
255.N	3.164674	6.087852	6.488540
256.H	-6.721748	3.791759	6.596941
257.N	1.068646	5.277596	6.535379
258.C	1.980393	4.221651	6.534662

Table S27 Cartesian coordinates (in Å) and ADF total bonding energy (in kcal/mol) of **G_4–K^+–G_4–K^+–G_4–K^+–G_4** at the ZORA-BLYP-D3(BJ)/TZP level of theory with COSMO to simulate water.

G_4–K^+–G_4–K^+–G_4–K^+–G_4 (Bond Energy: -39774.11 kcal/mol)			
1.C	-5.836839	-3.006045	3.329609
2.N	-4.530148	-2.804771	3.338126
3.C	-4.372997	-1.418493	3.342093
4.C	-3.205242	-0.618645	3.334061
5.O	-1.999914	-1.009368	3.322447
6.N	-3.494788	0.758734	3.333059
7.C	-4.776394	1.297818	3.332701
8.N	-4.884531	2.636342	3.348551
9.N	-5.884542	0.539116	3.318821
10.C	-5.629577	-0.781604	3.331616
11.C	4.226808	-3.812838	-0.082879
12.H	0.376880	-7.763929	-3.216281
13.N	0.645682	-6.783838	-3.237133
14.H	4.676512	6.210024	0.065532
15.N	3.843742	5.627354	0.056223
16.C	2.529612	6.074405	0.073349
17.C	1.941377	-6.289657	-3.248022
18.H	-6.331995	-3.968035	3.323845
19.H	-2.661778	1.383954	3.340193
20.H	-4.071257	3.284741	3.379676
21.H	-5.822525	3.018450	3.361184
22.N	1.970248	-4.966749	-3.293787
23.H	7.747283	0.477324	-3.230553
24.N	6.767171	0.746791	-3.236828
25.C	6.273457	2.042381	-3.208167
26.N	1.664498	5.075209	0.051873
27.C	2.069188	2.552716	-0.022744
28.N	4.950266	2.072853	-3.244274
29.C	4.557937	0.734727	-3.292279
30.C	3.265305	0.149333	-3.329568
31.O	2.149474	0.741089	-3.338625
32.N	3.315429	-1.259345	-3.351129
33.H	-6.211296	4.692659	0.194219
34.H	3.459897	-3.856205	-3.357147
35.N	-5.628736	3.860401	0.161129
36.H	5.217479	-3.882870	-3.344270
37.H	5.255184	0.136334	-0.045408
38.N	3.180763	1.690197	-0.043615
39.N	2.688947	4.889712	3.274198
40.H	6.417625	1.473469	-0.015027
41.C	4.506782	2.108357	-0.026532
42.C	2.441943	3.917575	0.022745
43.O	0.897123	2.072132	-0.046101
44.H	7.616587	1.673251	3.188081
45.N	6.605338	1.767418	3.227649
46.C	5.893809	2.957989	3.282269
47.N	4.587719	2.755565	3.315284
48.C	4.482974	-2.008187	-3.378988
49.C	4.430837	1.369667	3.281577
50.H	-2.920610	7.027408	-2.999742
51.C	-6.075970	2.546298	0.148943
52.N	-5.077091	1.681764	0.102770
53.O	-0.954625	2.003382	3.348181
54.C	1.350494	4.781061	3.295679
55.N	4.361602	-3.351125	-3.462347
56.N	0.812289	3.499192	3.311557
57.C	3.263159	0.569671	3.276081
58.H	6.927596	2.903348	-3.159423

59.C	3.811773	4.245576	0.025069
60.H	2.392060	-1.740550	-3.373905
61.O	2.057906	0.959873	3.302619
62.N	3.552539	-0.806824	3.228255
63.N	0.591088	5.888785	3.301130
64.C	-0.728572	5.633131	3.352394
65.N	5.455240	1.157713	-0.028060
66.N	5.705849	-1.456256	-3.352469
67.C	4.833738	-1.344829	3.180924
68.C	5.683432	-0.108632	-3.294858
69.N	4.941923	-2.683187	3.152923
70.N	5.941242	-0.585250	3.162544
71.C	-3.919441	2.459679	0.087227
72.C	-2.554873	2.087917	0.029921
73.H	1.723990	-7.610936	3.148798
74.N	1.819064	-6.599653	3.185203
75.C	3.010562	-5.887948	3.205774
76.N	2.808986	-4.581807	3.242483
77.C	1.422677	-4.425066	3.246807
78.C	0.622760	-3.257456	3.260963
79.O	1.013620	-2.052174	3.276464
80.N	-0.754533	-3.546881	3.249270
81.C	-1.293489	-4.828224	3.218934
82.N	-2.632053	-4.936634	3.227385
83.N	-0.534605	-5.935770	3.183645
84.C	0.786054	-5.681128	3.206911
85.O	-2.074661	0.916519	-0.020419
86.N	-1.692081	3.199456	0.031320
87.C	-2.109912	4.524813	0.079898
88.N	-1.159027	5.472902	0.096220
89.N	-3.405020	4.878554	0.114976
90.C	-4.247096	3.829090	0.123040
91.C	5.686755	0.734316	3.222388
92.H	3.972832	-6.382403	3.191875
93.H	-1.380033	-2.714294	3.273072
94.H	-3.280785	-4.124341	3.273657
95.H	-3.014049	-5.874721	3.218520
96.C	0.631200	-4.574957	-3.307051
97.C	0.044480	-3.282642	-3.334907
98.O	0.635246	-2.166543	-3.364638
99.H	7.109516	-2.283718	-0.082830
100.H	0.654211	-2.952846	-0.081641
101.H	0.117577	-5.257332	-0.040820
102.H	-7.129140	2.299595	0.174161
103.H	-0.676552	2.969918	-0.004890
104.H	-0.137631	5.272975	0.077826
105.H	-1.474421	6.434665	0.136254
106.H	-4.695973	-6.195529	0.026917
107.N	-3.863595	-5.612336	0.015043
108.C	-2.549346	-6.059109	-0.003170
109.N	-1.684782	-5.059363	-0.018997
110.C	-2.462719	-3.901687	-0.007803
111.C	-2.090933	-2.535999	-0.028433
112.O	-0.919556	-2.054510	-0.063502
113.N	-3.202608	-1.673602	-0.008348
114.C	-4.528064	-2.092595	0.024877
115.N	-5.476195	-1.142491	0.064650
116.N	-4.881801	-3.388210	0.023021
117.C	-3.832243	-4.230140	0.013365
118.H	1.455231	-6.419459	-0.050570
119.H	6.388438	3.920200	3.294636
120.H	2.719955	-1.432603	3.238447
121.H	4.129779	-3.332457	3.193390
122.H	5.879993	-3.065056	3.137767
123.N	-1.364231	-3.333270	-3.317783
124.C	-2.113087	-4.501265	-3.317925
125.H	-2.302710	-7.112616	-0.005303
126.H	-2.973036	-0.657478	-0.017022
127.H	-5.276079	-0.121058	0.076223
128.H	-6.438119	-1.458690	0.092380
129.N	-3.457636	-4.381019	-3.363543
130.N	-1.560059	-5.723873	-3.298987
131.C	-0.211444	-5.700690	-3.278882
132.H	-0.494463	7.848080	-3.045166
133.N	-0.763996	6.868471	-3.076171
134.C	-2.059624	6.374347	-3.061385

135.N	-2.090037	5.052336	-3.128177
136.C	-0.751836	4.661106	-3.182884
137.C	-0.166336	3.369626	-3.247027
138.O	-0.758008	2.254200	-3.281005
139.H	-7.863807	-0.396139	-3.046667
140.N	-6.884299	-0.664773	-3.086933
141.C	-6.390217	-1.960295	-3.111722
142.N	-5.068507	-1.988656	-3.184426
143.C	-4.677299	-0.649494	-3.202246
144.C	-3.385960	-0.062377	-3.254389
145.O	-2.270580	-0.652807	-3.308189
146.N	-3.436601	1.346291	-3.232361
147.C	-4.604459	2.094811	-3.205087
148.N	-4.485525	3.439430	-3.246341
149.N	-5.826384	1.541384	-3.162890
150.C	-5.802436	0.192772	-3.148432
151.N	1.242363	3.420238	-3.265121
152.N	-6.548544	-1.814410	3.327096
153.C	-2.952299	5.839162	3.415025
154.C	0.091543	5.786342	-3.157529
155.K	0.010459	-0.005468	1.632124
156.K	-0.040424	0.024742	-1.847149
157.H	2.803650	-6.943212	-3.218621
158.H	-7.042948	-2.822810	-3.071932
159.H	-2.513956	1.828539	-3.263063
160.H	-3.580824	3.943123	-3.162926
161.H	-5.338472	3.967351	-3.095466
162.H	3.866156	5.321681	-3.207125
163.H	1.723571	2.497576	-3.307561
164.H	-1.846031	-2.409996	-3.330293
165.H	-3.985936	-5.236559	-3.229220
166.H	-3.960841	-3.478298	-3.257768
167.H	-1.667313	7.563438	3.361051
168.H	6.192079	-4.676919	-0.096791
169.N	5.608962	-3.844431	-0.089112
170.C	6.055970	-2.530219	-0.080704
171.C	1.991329	4.588033	-3.263331
172.N	3.334420	4.468553	-3.343271
173.N	1.439287	5.810076	-3.210368
174.H	-3.914402	6.333614	3.437575
175.N	5.056364	-1.665354	-0.073235
176.C	3.898530	-2.443109	-0.073360
177.H	2.950612	0.674581	-0.072335
178.H	1.438014	2.666580	3.303852
179.H	3.338140	4.076869	3.296357
180.H	3.070910	5.827846	3.280609
181.C	2.532761	-2.070738	-0.080724
182.O	2.051280	-0.898890	-0.089528
183.N	-1.761622	6.551555	3.377365
184.H	3.839617	3.564378	-3.263418
185.H	2.283293	7.127631	0.099896
186.N	1.670321	-3.182591	-0.080080
187.C	2.089178	-4.508464	-0.076698
188.H	-7.560371	-1.719070	3.313979
189.N	-2.750076	4.532639	3.418287
190.C	-1.364219	4.376251	3.381918
191.C	-0.564317	3.208875	3.350590
192.N	1.139069	-5.457128	-0.053000
193.N	3.384679	-4.862290	-0.090791
194.N	4.860992	3.403615	-0.003753
195.C	-6.322981	1.757525	6.572879
196.N	-5.233415	1.005817	6.592046
197.C	-4.169667	1.909027	6.618170
198.C	-2.767911	1.688695	6.612819
199.O	-2.160770	0.581043	6.603847
200.N	-2.035796	2.893653	6.606969
201.C	-2.599443	4.161046	6.637931
202.N	-1.759848	5.216036	6.688080
203.N	-3.925714	4.371084	6.640526
204.C	-4.647574	3.231834	6.619494
205.H	-7.343175	1.397089	6.545185
206.H	-0.999956	2.788212	6.606443
207.H	-0.728165	5.140967	6.597067
208.H	-2.183477	6.132404	6.592744
209.N	5.340592	1.770354	6.573032
210.H	6.825000	-3.985141	6.305934

211.N	6.154830	-3.222232	6.350830
212.C	6.453541	-1.868080	6.356828
213.N	5.365344	-1.117615	6.428920
214.C	4.302738	-2.021750	6.467104
215.O	0.704698	2.170896	6.590042
216.C	4.284440	2.609846	6.542515
217.N	3.016762	2.046156	6.543070
218.C	2.901506	-1.802112	6.512092
219.O	2.294398	-0.695035	6.549049
220.N	2.169364	-3.007038	6.499953
221.N	4.494434	3.935999	6.534590
222.C	3.354966	4.657810	6.536050
223.C	2.733501	-4.274514	6.481278
224.N	1.895579	-5.331082	6.530710
225.N	4.059052	-4.483709	6.437735
226.H	-3.863747	-6.815972	6.408494
227.N	-3.100470	-6.145266	6.436106
228.C	-1.746286	-6.443366	6.416114
229.N	-0.995091	-5.354545	6.468475
230.C	-1.898814	-4.292188	6.520406
231.C	-1.678922	-2.890786	6.554963
232.O	-0.571388	-2.283386	6.568190
233.N	-2.884086	-2.158982	6.562562
234.C	-4.151514	-2.723589	6.572362
235.N	-5.207021	-1.885896	6.638769
236.N	-4.360976	-4.049518	6.538704
237.C	-3.221452	-4.770296	6.503089
238.C	4.780139	-3.343920	6.421449
239.H	-1.385236	-7.462173	6.360876
240.H	-2.778857	-1.123385	6.587491
241.H	-5.131784	-0.851958	6.578909
242.H	-6.122901	-2.306937	6.528641
243.H	7.472356	-1.506718	6.304045
244.H	1.133974	-2.902007	6.531463
245.H	0.861899	-5.253815	6.467383
246.H	2.316082	-6.243939	6.395525
247.N	-6.023882	3.111540	6.590073
248.C	1.880097	6.333185	6.514634
249.K	0.050366	-0.044995	5.106186
250.H	3.997505	6.704572	6.475856
251.H	1.519354	7.353317	6.489384
252.H	2.911385	1.010345	6.547956
253.H	5.263151	0.739032	6.479250
254.H	6.253740	2.193967	6.449991
255.N	3.234122	6.033942	6.502146
256.H	-6.694826	3.875109	6.584105
257.N	1.128988	5.243868	6.556590
258.C	2.032470	4.180075	6.567274
259.C	1.812101	2.778249	6.572561