Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Quantitative analysis of molecular surface: systematic application on sodiation mechanism of benzoquinone-based pillared compound as cathode

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8. References

1. Properties of pillar[5]quinone molecular.

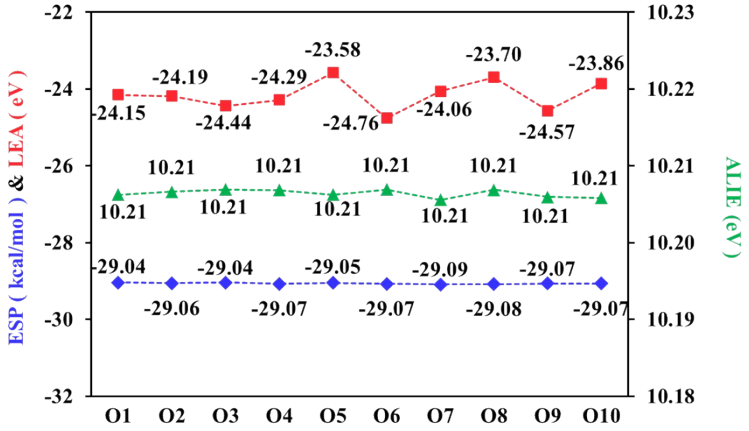

Fig. S1 Quantitative analysis of P5Q molecular surface.

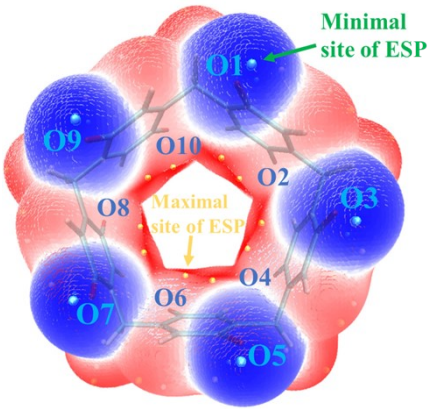

Fig. S2 Minimal sites of the electrostatic potential on the vdW surface of P5Q.

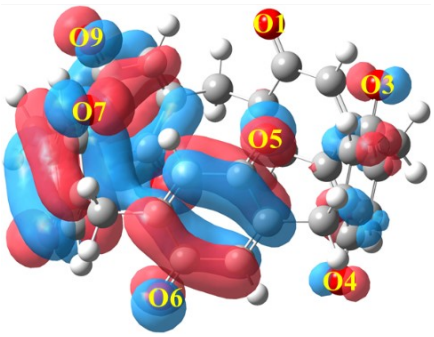

Fig. S3 Distribution of LUMO orbitals of P5Q.

2. Definition and application of root-mean-square deviation.

The root-mean-square deviation (RMSD) between the structures of the reactants and products before and after the redox reaction can be calculated by the VMD software to measure the degree of structural deformation of the molecule,[1, 2] defined as:

$$\mathrm{RMSD} = \sqrt{\frac{1}{\mathrm{N}}\sum_{i}^{\mathrm{natom}}\left[(x_i - x_i')^2 + (y_i - y_i')^2 + (z_i - z_i')^2\right]}$$

Under the assumption that the decay of battery capacity is mainly due to the dissolution of reduction products in the electrolyte, the P5QNa$_n$ (n = 1–10) during the discharge process should not show excessive deformation because P5Q has good cyclability as an electrode material. Therefore, the molecular deformation of the sodiated structures should be as imperceptible as possible to keep the reaction site of P5Q spatially unobstructed, maintain the reactivity, and maximize the conformational advantages of the pillared compounds.

3. Interaction region indicator analyses.

The Interaction region indicator (IRI) functions of isomers P5QNa$_2$ and P5QNa$_3$ were calculated via Multiwfn, and the results were imported to VMD to render the chemical bonding and weak interaction regions.[3] From the mapped colors of IRI isosurfaces, it is intuitively visualized the interactions between the different atoms in Fig. S4.

$$\mathrm{IRI}(r) = \frac{|\nabla\rho(r)|}{[\rho(r)]^{\mathrm{a}}}$$

where a is an adjustable parameter, a =1.1 is adopted for the standard definition of IRI. IRI is essentially the gradient norm of electron density-weighted by scaled electron

density. As will be shown, isosurfaces of IRI can exhibit various kinds of interaction regions.[4]

As shown in Fig. S5, Na1 (Na2) in P5QNa$_2$/O6 forms a high interaction with O5 (O6) (ionic bond, bond length 2.25 Å of O5–Na1, chemisorption), which is shown as a light blue color. For comparison, weak interaction between the positively charged Na1 and the negatively charged O3 (Na1···O3 distance of 3.65 Å, physisorption) appeared green color. Na1 in P5QNa$_2$/O4, which is closer to O3 (2.81 Å) and produces a broader range of weak interactions, even has a weak repulsive effect with the nearest carbon atom. P5QNa$_2$/O4 showed more prominent chelating effects due to the distortion of the molecular framework, which leads to a reduced potential for the subsequent sodiation products to maintain excellent recyclability. Consequently, the physicochemical properties of the molecules are considered more important than the regularity of the computational software when conducting theoretical studies.

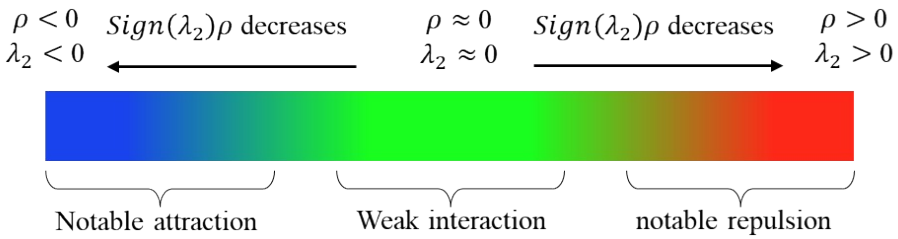

Fig. S4 Standard coloring method and chemical explanation of sign(λ_2)ρ on IRI isosurfaces.

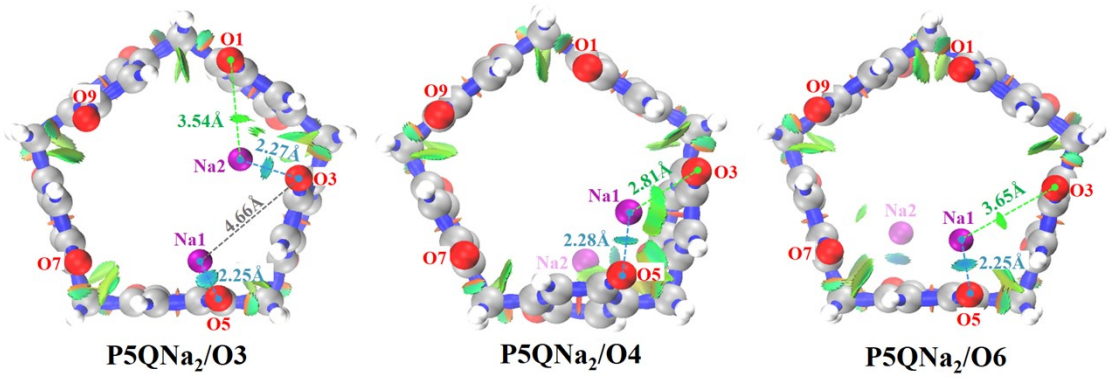

Fig. S5 Isosurface map of IRI of P5QNa$_2$/O3, P5QNa$_2$/O4, and P5QNa$_2$/O6.

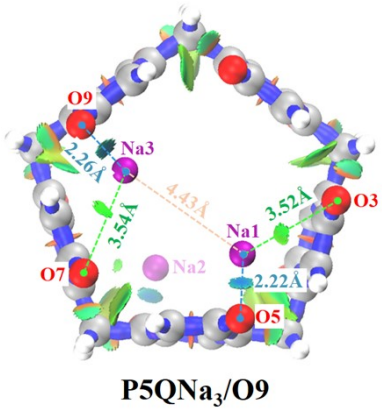

Fig. S6 Isosurface map of IRI of P5QNa$_3$/O9.

4. Properties of P5QNa$_2^-$ anion.

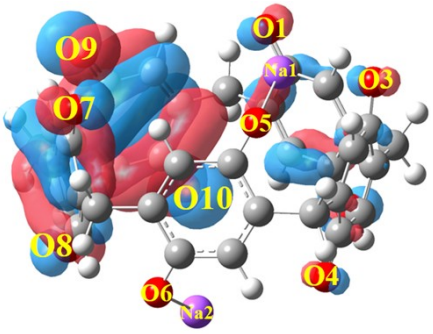

Fig. S7 Distribution of HOMO orbitals of P5QNa$_2^-$ anion.

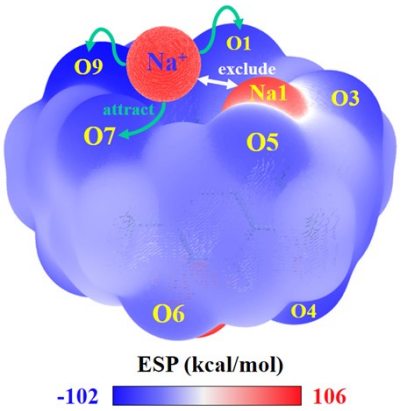

Fig. S8 Electrostatic potential of $P5QNa_2^-$ anion.

5. LUMO and HOMO orbitals distribution of P5QNa$_n$ (n = 0–10).

As shown in Fig 7, the E_{LUMO} was lowest at the beginning of the sodiation process (–3.66 eV) and gradually increased with the decrease of discharge voltage. When the 10th Na^+ was intercalated into P5Q molecule, the E_{LUMO} raised dramatically to –0.59 eV, resulting in weaker electron–binding and oxidation ability of $P5QNa_{10}$ with the discharge voltage no longer decreased. It was also evident from the LUMO orbitals distribution that the molecular framework of $P5QNa_{10}$ did not provide empty orbitals that could be occupied by free electrons (Fig S9).[5] The trend of E_{HOMO} was different from that of E_{LUMO}. P5Q and $P5QNa_1$ are difficult to provide electrons because of the substantial negative E_{HOMO} compared to the subsequent discharge products. However, the E_{HOMO} steadily increased after the E_{HOMO} of $P5QNa_2$ rapidly reached –3.91 eV. And the E_{HOMO} of P5QNa$_n$ (n = 2–10) remained between –3.91 and –3.25 eV, predicting the stable reducing ability of the sodiated product (Fig. 7).

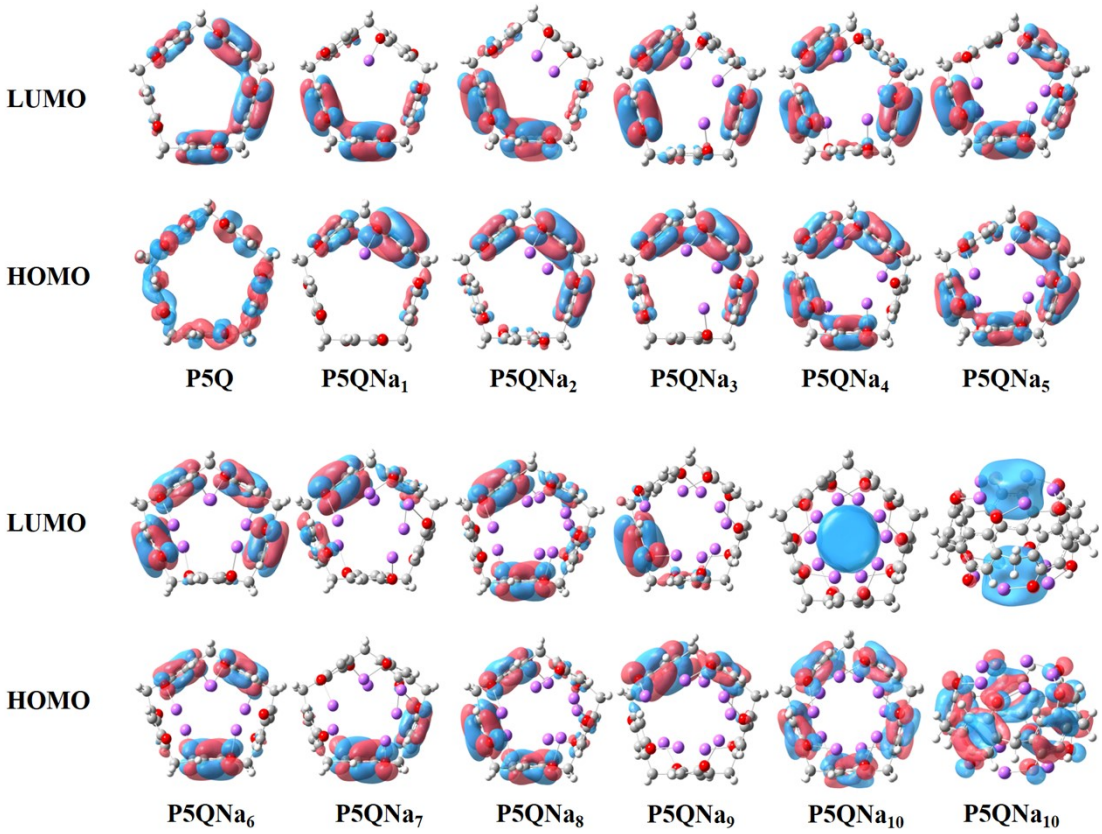

Fig. S9 LUMO and HOMO orbitals distribution of P5QNa$_n$ (n = 0–10).

6. The discharge-charge curves of pristine P5Q.

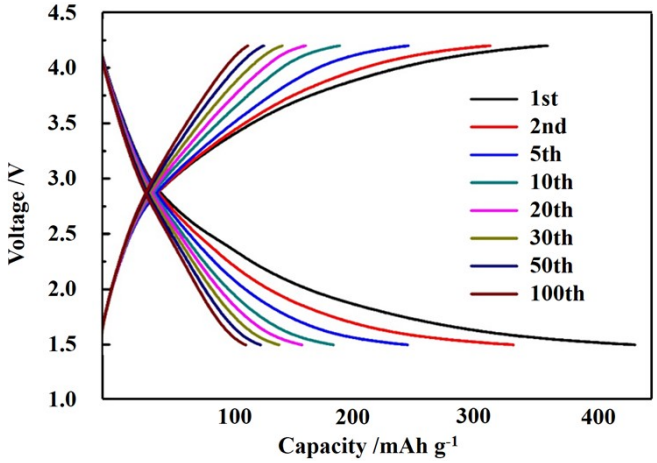

Fig. S10 The discharge-charge curves of pristine P5Q.

7. The DFT calculation results of sodiated products P5QNa*n* (*n* = 0–10).

Table S1 Optimized geometry of P5Q. (Single-point Energy = –2098.118900 Hartree, Gibbs Free Energy = –2098.212052 Hartree).

Serial number	Symbol	X	Y	Z
1	C	0.557503	–4.120490	1.213271
2	C	1.958204	–3.656370	1.239846
3	C	2.660031	–3.442728	–0.063887
4	C	1.993006	–3.646187	–1.213847
5	C	0.589965	–4.103046	–1.240393
6	C	–0.101097	–4.349554	0.063261
7	H	0.080192	–4.258202	2.177761
8	H	2.458316	–3.472119	–2.178321
9	O	2.532891	–3.450877	2.306755
10	O	0.004695	–4.276147	–2.307295
11	C	–0.127661	4.347481	–0.062647
12	C	0.565503	4.105368	1.240774
13	C	2.639582	3.459223	0.063453
14	C	1.935681	3.667777	–1.240015
15	C	0.531926	4.122515	–1.212895
16	H	0.053413	4.257202	–2.177217
17	O	–0.020535	4.274671	2.307870
18	O	2.511253	3.465983	–2.307147
19	C	–4.177838	1.222348	–0.063316
20	C	–3.733134	1.805304	1.240639
21	C	–2.871574	3.003207	1.214657
22	C	–2.475279	3.577658	0.065016
23	C	–2.892549	2.974879	–1.239017
24	C	–3.759979	1.781175	–1.213024
25	H	–2.564065	3.393048	2.179275
26	H	–4.036243	1.368762	–2.177709
27	O	–4.076016	1.299902	2.307320
28	O	–2.522211	3.460495	–2.305698
29	C	–2.452618	–3.592752	–0.064370
30	C	–2.871477	–2.990762	1.239501
31	C	–3.746502	–1.802612	1.213307
32	C	–4.169318	–1.247646	0.063540
33	C	–3.721818	–1.828647	–1.240324
34	C	–2.853472	–3.021694	–1.214135
35	H	–4.024369	–1.391040	2.177878
36	H	–2.545204	–3.410900	–2.178764
37	O	–2.497368	–3.473296	2.306261

38	O	–4.068616	–1.326114	–2.307085
39	C	4.091327	–0.742718	1.213273
40	C	4.083554	0.732813	1.239427
41	C	4.097830	1.465959	–0.064502
42	C	4.085721	0.768433	–1.214295
43	C	4.086389	–0.707105	–1.240439
44	C	4.106245	–1.440175	0.063473
45	H	4.074012	–1.239019	2.177840
46	H	4.064592	1.264618	–2.178854
47	O	4.065221	1.343217	2.306141
48	O	4.070888	–1.317569	–2.307168
49	C	–1.570865	4.784247	0.001726
50	H	–1.719776	5.396266	0.892204
51	H	–1.813515	5.366609	–0.888028
52	C	–5.038758	–0.015617	–0.000016
53	H	–5.667531	0.031069	0.890026
54	H	–5.666817	–0.066668	–0.890294
55	C	–1.541787	–4.794516	–0.000645
56	H	–1.687528	–5.407888	–0.890732
57	H	–1.781074	–5.377697	0.889487
58	C	4.084379	–2.947864	0.000017
59	H	4.622806	–3.276149	–0.889933
60	H	4.564914	–3.355459	0.890317
61	C	4.067025	2.973495	–0.001045
62	H	4.544661	3.384017	–0.891559
63	H	4.603805	3.305069	0.888697
64	C	1.971710	3.658380	1.213684
65	H	2.438662	3.487679	2.177967

Table S2 Optimized geometry of $P5QNa_1$ (Single-point Energy = –2260.525262 Hartree, Gibbs Free Energy = –2260.630227 Hartree).

Serial number	Symbol	X	Y	Z
1	C	4.247098	–0.351285	–1.238824
2	C	3.879274	–1.780075	–1.218797
3	C	3.678090	–2.442478	0.107634
4	C	3.830640	–1.724438	1.234276
5	C	4.213002	–0.299500	1.214310
6	C	4.422449	0.361247	–0.111547
7	H	4.362485	0.100126	–2.218639
8	H	3.669517	–2.163489	2.213148
9	O	3.741603	–2.409864	–2.265361
10	O	4.353112	0.327632	2.262400
11	C	–4.326109	–0.150706	–0.225288
12	C	–3.886015	–0.776447	–1.505623
13	C	–3.225608	–2.838688	–0.307859
14	C	–3.621045	–2.190550	0.979113
15	C	–4.218751	–0.853776	0.922287
16	H	–4.531024	–0.423772	1.866885
17	O	–3.987791	–0.180693	–2.578945
18	O	–3.435921	–2.765329	2.057292
19	C	–1.420730	4.003138	–0.079640
20	C	–2.005113	3.694424	–1.387588
21	C	–3.143284	2.798549	–1.389643
22	C	–3.635260	2.215445	–0.251548
23	C	–2.987591	2.456101	1.030278
24	C	–1.890740	3.392597	1.049777
25	H	–3.596895	2.586551	–2.352955
26	H	–1.430023	3.595829	2.012913
27	O	–1.545081	4.193172	–2.451485
28	O	–3.373795	1.860836	2.092978
29	C	3.501091	2.651405	–0.024409
30	C	2.846033	3.008941	–1.322659
31	C	1.607068	3.799682	–1.280981
32	C	1.037586	4.193382	–0.123738
33	C	1.661147	3.782747	1.172248
34	C	2.921460	3.017782	1.132533
35	H	1.154702	4.046347	–2.236062
36	H	3.349113	2.745394	2.091693
37	O	3.341421	2.652425	–2.392507
38	O	1.139093	4.070022	2.249255
39	C	1.129605	–4.086663	–1.233405

40	C	–0.340218	–4.157917	–1.340275
41	C	–1.144676	–4.154369	–0.078652
42	C	–0.515763	–4.029802	1.104303
43	C	0.951961	–3.930145	1.209421
44	C	1.759396	–3.995623	–0.048675
45	H	1.679339	–4.097662	–2.168502
46	H	–1.069754	–3.990017	2.036546
47	O	–0.888435	–4.219008	–2.438696
48	O	1.499012	–3.797312	2.302794
49	C	–4.818884	1.269841	–0.277416
50	H	–5.392664	1.425408	–1.193131
51	H	–5.459250	1.459315	0.587244
52	C	–0.252754	4.964746	–0.053393
53	H	–0.325580	5.626018	–0.918219
54	H	–0.269827	5.552198	0.866237
55	C	4.765706	1.829931	–0.097206
56	H	5.388893	2.043995	0.772347
57	H	5.306980	2.085355	–1.008867
58	C	3.258535	–3.891533	0.092346
59	H	3.565087	–4.367823	1.024491
60	H	3.736533	–4.393950	–0.749776
61	C	–2.643871	–4.229463	–0.223740
62	H	–3.066688	–4.740724	0.641991
63	H	–2.886708	–4.782193	–1.132117
64	C	–3.341803	–2.148386	–1.458037
65	H	–3.030807	–2.574113	–2.406793
66	Na	–1.968247	0.542134	3.250206

Table S3 Optimized geometry of $P5QNa_2$ (Single-point Energy = –2422.918009 Hartree, Gibbs Free Energy = –2423.035588 Hartree).

Serial number	Symbol	X	Y	Z
1	C	3.421077	–2.429794	1.093071
2	C	4.062870	–1.108499	1.175252
3	C	4.439876	–0.427046	–0.101344
4	C	4.167209	–1.023159	–1.276567
5	C	3.522020	–2.345039	–1.357832
6	C	3.169633	–3.039430	–0.083001
7	H	3.153817	–2.897344	2.035280
8	H	4.396603	–0.541731	–2.221260
9	O	4.287387	–0.576711	2.264363
10	O	3.279168	–2.858712	–2.450708
11	C	–3.138504	2.888511	0.248378
12	C	–2.350613	2.999851	1.497318
13	C	–0.590956	4.238077	0.277295
14	C	–1.327984	4.023421	–0.996008
15	C	–2.640492	3.400122	–0.909247
16	H	–3.211455	3.325230	–1.828474
17	O	–2.752296	2.514572	2.569519
18	O	–0.833865	4.372994	–2.085932
19	C	–3.605894	–2.105774	–0.181088
20	C	–3.626451	–1.543024	1.161813
21	C	–3.953321	–0.150541	1.275245
22	C	–4.129455	0.663509	0.179084
23	C	–3.940386	0.132812	–1.163195
24	C	–3.735233	–1.282970	–1.276971
25	H	–4.031897	0.267291	2.274260
26	H	–3.654009	–1.699843	–2.276262
27	O	–3.368391	–2.267108	2.190805
28	O	–3.962959	0.901494	–2.192059
29	C	0.986737	–4.170216	–0.284637
30	C	0.223015	–4.224001	0.990128
31	C	–1.225938	–4.113588	0.904321
32	C	–1.876125	–3.824379	–0.254068
33	C	–1.102092	–3.653999	–1.505281
34	C	0.345313	–3.882561	–1.440867
35	H	–1.784337	–4.232342	1.826390
36	H	0.892458	–3.793126	–2.374170
37	O	0.810586	–4.362152	2.080590
38	O	–1.652349	–3.351308	–2.578141
39	C	3.510435	2.453254	1.281352

40	C	2.430896	3.452726	1.358068
41	C	1.853986	3.970264	0.080884
42	C	2.312305	3.491267	–1.093200
43	C	3.390166	2.493008	–1.170953
44	C	3.984397	1.995555	0.108025
45	H	3.895511	2.088471	2.227634
46	H	1.896796	3.829395	–2.037037
47	O	2.016988	3.846677	2.449251
48	O	3.796141	2.078149	–2.258337
49	C	–4.439638	2.136856	0.316292
50	H	–4.928857	2.327502	1.273887
51	H	–5.091628	2.456047	–0.500106
52	C	–3.360713	–3.591338	–0.319697
53	H	–3.852111	–4.125411	0.496853
54	H	–3.749465	–3.945413	–1.276805
55	C	2.482362	–4.374182	–0.199202
56	H	2.836090	–4.882338	–1.097786
57	H	2.708113	–4.978494	0.680296
58	C	5.061765	0.943795	0.005325
59	H	5.667191	1.136191	–0.881615
60	H	5.692323	0.983671	0.894712
61	C	0.730967	4.966978	0.192415
62	H	0.724783	5.609615	–0.688799
63	H	0.875938	5.570853	1.089738
64	C	–1.081906	3.732028	1.432409
65	H	–0.535662	3.839777	2.364283
66	Na	–1.485138	–1.810628	3.330830
67	Na	–2.031177	1.185527	–3.301459

Table S4 Optimized geometry of $P5QNa_3$ (Single-point Energy = –2585.321146 Hartree, Gibbs Free Energy = –2585.448788 Hartree).

Serial number	Symbol	X	Y	Z
1	C	4.205845	0.275606	–1.350790
2	C	4.092857	–1.168315	–1.379839
3	C	4.006718	–1.838151	–0.083122
4	C	3.969899	–1.106013	1.073798
5	C	4.034028	0.330527	1.090272
6	C	4.194202	1.004749	–0.190004
7	H	4.289105	0.779798	–2.309542
8	H	3.869590	–1.609338	2.031491
9	O	4.076819	–1.815818	–2.465677
10	O	3.941319	0.988584	2.188077
11	C	–4.237713	–0.971497	–0.168808
12	C	–3.634086	–1.408973	–1.445261
13	C	–2.669869	–3.382454	–0.303293
14	C	–3.187275	–2.884908	0.996365
15	C	–4.027292	–1.700651	0.963483
16	H	–4.477798	–1.390302	1.900739
17	O	–3.785028	–0.762570	–2.500863
18	O	–2.907450	–3.469493	2.065945
19	C	–2.125571	3.569250	0.121726
20	C	–2.548871	3.112198	–1.192912
21	C	–3.539884	2.081401	–1.227078
22	C	–3.993956	1.443262	–0.091100
23	C	–3.443050	1.785639	1.208469
24	C	–2.543210	2.903873	1.252871
25	H	–3.911764	1.772584	–2.199051
26	H	–2.170725	3.211497	2.226126
27	O	–2.044425	3.614730	–2.267447
28	O	–3.762508	1.127280	2.267363
29	C	2.919900	3.130026	–0.066790
30	C	2.160897	3.425332	–1.315017
31	C	0.840435	4.036999	–1.173241
32	C	0.236741	4.218131	0.029140
33	C	0.954244	3.823907	1.266206
34	C	2.337512	3.364729	1.130803
35	H	0.326018	4.316826	–2.086064
36	H	2.876574	3.145833	2.045399
37	O	2.645460	3.180049	–2.432411
38	O	0.407973	3.879919	2.381966
39	C	1.789479	–3.870640	–1.360078

40	C	0.357107	–4.173198	–1.444683
41	C	–0.401445	–4.351589	–0.168879
42	C	0.230393	–4.169338	1.009003
43	C	1.658576	–3.831726	1.092421
44	C	2.431001	–3.718092	–0.181677
45	H	2.319362	–3.744816	–2.298286
46	H	–0.304902	–4.259384	1.949057
47	O	–0.208983	–4.284297	–2.537317
48	O	2.203639	–3.654349	2.186793
49	C	–5.004343	0.321630	–0.167911
50	H	–5.589832	0.411244	–1.086025
51	H	–5.672159	0.353763	0.696471
52	C	–1.167270	4.738676	0.177881
53	H	–1.389100	5.428323	–0.639771
54	H	–1.265078	5.257044	1.133768
55	C	4.291562	2.516670	–0.193491
56	H	4.906962	2.841013	0.649704
57	H	4.751335	2.851077	–1.125172
58	C	3.886244	–3.345627	–0.082827
59	H	4.305096	–3.757396	0.837263
60	H	4.420889	–3.746109	–0.945844
61	C	–1.870242	–4.664914	–0.281854
62	H	–2.182592	–5.261286	0.576619
63	H	–2.044734	–5.222547	–1.203513
64	C	–2.873982	–2.660481	–1.432020
65	H	–2.463484	–2.990274	–2.381734
66	Na	–0.895694	2.089138	–3.463006
67	Na	–2.295218	–0.212867	3.265214
68	Na	1.999569	0.865905	3.331098

Table S5 Optimized geometry of $P5QNa_4$ (Single-point Energy = –2747.710433 Hartree, Gibbs Free Energy = –2747.842136 Hartree).

Serial number	Symbol	X	Y	Z
1	C	3.352849	1.993058	1.247090
2	C	2.456754	3.106973	1.103145
3	C	2.258403	3.609110	–0.246158
4	C	2.798910	2.934797	–1.321714
5	C	3.615666	1.770703	–1.183251
6	C	3.951466	1.365092	0.176896
7	H	3.560437	1.649173	2.257230
8	H	2.593648	3.282856	–2.329249
9	O	1.883975	3.650381	2.119281
10	O	4.040197	1.116312	–2.209055
11	C	–4.108943	–1.608173	0.353355
12	C	–3.732463	–0.788287	1.520645
13	C	–4.078598	1.259143	0.166858
14	C	–4.305999	0.422709	–1.032852
15	C	–4.431453	–1.001742	–0.826395
16	H	–4.702099	–1.607607	–1.684301
17	O	–3.406204	–1.301519	2.612378
18	O	–4.354855	0.930158	–2.183697
19	C	0.186372	–4.133287	–0.170144
20	C	–0.317770	–3.986361	1.190856
21	C	–1.705944	–3.681215	1.329914
22	C	–2.535773	–3.430649	0.255622
23	C	–1.992005	–3.402230	–1.092094
24	C	–0.619838	–3.805621	–1.237450
25	H	–2.107527	–3.638153	2.337587
26	H	–0.222513	–3.858415	–2.248092
27	O	0.448894	–4.133756	2.216796
28	O	–2.706620	–3.064761	–2.106729
29	C	4.175738	–1.079562	0.168075
30	C	3.570390	–1.756053	1.329832
31	C	2.929151	–3.037545	1.078701
32	C	2.550964	–3.441824	–0.164963
33	C	2.983219	–2.645502	–1.329010
34	C	3.949985	–1.589004	–1.074718
35	H	2.611052	–3.617724	1.936547
36	H	4.390492	–1.094063	–1.931467
37	O	3.583636	–1.260231	2.483999
38	O	2.533741	–2.841911	–2.485765
39	C	–0.728792	4.445385	0.830588

40	C	–2.019947	3.820520	1.020606
41	C	–2.694412	3.285791	–0.185261
42	C	–2.017932	3.223147	–1.360716
43	C	–0.646282	3.709859	–1.513801
44	C	–0.034232	4.366290	–0.340812
45	H	–0.278802	4.928454	1.691351
46	H	–2.486030	2.784116	–2.237391
47	O	–2.539488	3.711245	2.158769
48	O	–0.039671	3.600770	–2.599848
49	C	–3.996564	–3.101981	0.462439
50	H	–4.319128	–3.444190	1.448379
51	H	–4.610085	–3.578212	–0.307409
52	C	1.613233	–4.603803	–0.368801
53	H	1.842612	–5.386038	0.360972
54	H	1.732225	–5.006264	–1.376762
55	C	4.918639	0.215283	0.371244
56	H	5.727116	0.289260	–0.362105
57	H	5.340031	0.251564	1.377907
58	C	1.390707	4.830175	–0.447849
59	H	1.580963	5.263429	–1.432446
60	H	1.596118	5.576013	0.324792
61	C	–4.097668	2.757020	–0.017417
62	H	–4.685645	2.994995	–0.905846
63	H	–4.548350	3.227062	0.858707
64	C	–3.789187	0.664626	1.353538
65	H	–3.565887	1.270204	2.227542
66	Na	1.010933	–2.179164	3.300280
67	Na	–2.547300	–1.099129	–3.197552
68	Na	2.465403	–0.134553	–3.332857
69	Na	0.153751	2.716388	3.200041

Table S6 Optimized geometry of $P5QNa_5$ (Single-point Energy = –2910.103673 Hartree, Gibbs Free Energy = –2910.248868 Hartree).

Serial number	Symbol	X	Y	Z
1	C	–4.421016	–1.365417	1.185419
2	C	–3.432969	–2.393674	1.372936
3	C	–2.947512	–3.055819	0.154725
4	C	–3.326239	–2.563930	–1.057487
5	C	–4.013502	–1.296914	–1.223368
6	C	–4.635021	–0.744892	–0.027199
7	H	–4.893178	–0.959519	2.071726
8	H	–2.969179	–3.069851	–1.947090
9	O	–2.980976	–2.684674	2.528317
10	O	–4.016302	–0.720279	–2.355287
11	C	4.537552	0.909902	0.174802
12	C	4.497947	–0.022578	1.309214
13	C	4.177461	–1.899227	–0.272632
14	C	4.071939	–0.958329	–1.376183
15	C	4.446185	0.413461	–1.091502
16	H	4.459560	1.110618	–1.921493
17	O	4.426503	0.379004	2.515333
18	O	3.617660	–1.263812	–2.526227
19	C	0.402171	3.933297	0.409275
20	C	1.042330	3.602067	1.678307
21	C	2.402529	3.116674	1.596186
22	C	3.065121	2.891538	0.413108
23	C	2.363440	3.090133	–0.849066
24	C	1.055758	3.681941	–0.769289
25	H	2.910389	2.924324	2.537809
26	H	0.569791	3.938824	–1.706340
27	O	0.453070	3.755590	2.792034
28	O	2.864630	2.760152	–1.987111
29	C	–4.196755	1.592497	0.020346
30	C	–3.596437	1.816218	1.327139
31	C	–2.544707	2.797561	1.397462
32	C	–2.062299	3.460251	0.298231
33	C	–2.557362	3.117317	–1.032051
34	C	–3.658852	2.211814	–1.095777
35	H	–2.121094	3.009032	2.376035
36	H	–4.074803	1.997480	–2.075572
37	O	–3.981701	1.186576	2.375855
38	O	–2.014735	3.618696	–2.090522
39	C	0.294120	–3.582949	1.146697

40	C	1.710436	–3.337128	1.035873
41	C	2.271080	–3.379522	–0.306177
42	C	1.420953	–3.416811	–1.396650
43	C	0.001359	–3.543102	–1.285492
44	C	–0.529755	–3.757900	0.062422
45	H	–0.111874	–3.671302	2.151763
46	H	1.837808	–3.378103	–2.398543
47	O	2.432326	–3.143685	2.077626
48	O	–0.764596	–3.515922	–2.320554
49	C	4.502200	2.398775	0.413433
50	H	4.962155	2.634895	1.375357
51	H	5.060404	2.906069	–0.379738
52	C	–0.989763	4.518514	0.428957
53	H	–1.126738	5.047474	1.375177
54	H	–1.095612	5.223841	–0.399394
55	C	–5.322910	0.592760	–0.101228
56	H	–5.844963	0.723575	–1.052019
57	H	–6.034655	0.700238	0.722454
58	C	–1.969418	–4.200351	0.247139
59	H	–2.208831	–4.932273	–0.531663
60	H	–2.066839	–4.682771	1.222053
61	C	3.771800	–3.333169	–0.478705
62	H	4.040353	–3.680389	–1.479353
63	H	4.259906	–3.969689	0.265816
64	C	4.486375	–1.424456	0.982427
65	H	4.575363	–2.128859	1.801029
66	Na	–0.748382	2.207835	–3.267335
67	Na	–2.733718	–0.420340	3.455471
68	Na	–1.579001	–1.528411	–3.169846
69	Na	2.645378	–1.177749	3.262539
70	Na	2.205502	0.743384	–2.992780

Table S7 Optimized geometry of $P5QNa_6$ (Single-point Energy = –3072.480335 Hartree, Gibbs Free Energy = –3072.633692 Hartree).

Serial number	Symbol	X	Y	Z
1	C	–0.588165	3.588823	–1.263360
2	C	0.835070	3.534012	–1.185456
3	C	1.395539	3.651921	0.142489
4	C	0.559441	3.594504	1.250443
5	C	–0.863684	3.532988	1.172686
6	C	–1.424726	3.645079	–0.155433
7	H	–1.028112	3.623537	–2.258272
8	H	0.999282	3.633626	2.245263
9	O	1.575458	3.434794	–2.256242
10	O	–1.603207	3.432907	2.243834
11	C	1.284406	–3.616086	–0.078970
12	C	1.824507	–3.276306	–1.384517
13	C	3.762747	–2.228325	–0.247078
14	C	3.148224	–2.430062	1.048613
15	C	1.930790	–3.190265	1.060330
16	H	1.514983	–3.451742	2.030269
17	O	1.186603	–3.579158	–2.475624
18	O	3.654012	–1.966985	2.144625
19	C	–3.741726	–2.249078	0.253689
20	C	–3.131899	–2.453605	–1.043444
21	C	–1.910796	–3.207434	–1.056274
22	C	–1.256224	–3.622914	0.082743
23	C	–1.792076	–3.279112	1.388581
24	C	–3.061094	–2.633419	1.403711
25	H	–1.499520	–3.473167	–2.027208
26	H	–3.509667	–2.431763	2.372476
27	O	–3.644882	–1.997998	–2.139800
28	O	–1.147894	–3.572493	2.479029
29	C	–3.659521	2.549792	–0.167908
30	C	–3.954369	1.710416	–1.332752
31	C	–4.673185	0.488251	–1.078654
32	C	–4.755551	–0.079853	0.172116
33	C	–4.326530	0.698457	1.330131
34	C	–3.960610	2.075882	1.078830
35	H	–4.993168	–0.091560	–1.936275
36	H	–3.740007	2.705550	1.933117
37	O	–3.562169	2.009118	–2.510299
38	O	–4.217901	0.210590	2.500686
39	C	3.941103	2.091952	–1.084661

40	C	4.319569	0.716690	–1.330044
41	C	4.757658	–0.051894	–0.169047
42	C	4.671393	0.521297	1.079293
43	C	3.941583	1.737738	1.328636
44	C	3.638102	2.569264	0.160069
45	H	3.713954	2.715981	–1.941414
46	H	4.999178	–0.050278	1.939526
47	O	4.213666	0.222656	–2.498144
48	O	3.547291	2.038530	2.504868
49	C	0.016253	–4.438376	0.001197
50	H	–0.030891	–5.071969	–0.888848
51	H	0.067023	–5.072931	0.890437
52	C	–5.077127	–1.540839	0.336332
53	H	–5.741109	–1.873380	–0.467463
54	H	–5.549594	–1.737849	1.301646
55	C	–2.919255	3.851710	–0.331139
56	H	–3.274857	4.560765	0.424865
57	H	–3.112122	4.269761	–1.322124
58	C	2.888918	3.866785	0.318108
59	H	3.078874	4.289492	1.307681
60	H	3.240718	4.575296	–0.440197
61	C	5.092946	–1.510418	–0.327380
62	H	5.756791	–1.834518	0.479932
63	H	5.570421	–1.706774	–1.290350
64	C	3.089669	–2.622866	–1.397905
65	H	3.541022	–2.423453	–2.365753
66	Na	–2.737801	–0.164409	–3.196924
67	Na	–0.066811	–1.902345	3.419418
68	Na	–2.022893	1.385161	3.136620
69	Na	2.008616	1.384359	–3.137141
70	Na	0.073687	–1.925582	–3.405241
71	Na	2.743448	–0.138872	3.203754

Table S8 Optimized geometry of $P5QNa_7$ (Single-point Energy = –3234.876351 Hartree, Gibbs Free Energy = –3235.036030 Hartree).

Serial number	Symbol	X	Y	Z
1	C	0.111677	3.672285	1.212919
2	C	–1.316650	3.478490	1.181492
3	C	–1.977273	3.633089	–0.112412
4	C	–1.203971	3.828593	–1.231871
5	C	0.229636	3.952921	–1.204426
6	C	0.868821	3.937929	0.100433
7	H	0.591351	3.615824	2.187155
8	H	–1.681167	3.917506	–2.204992
9	O	–1.957032	3.208475	2.256479
10	O	0.909118	4.084739	–2.286110
11	C	–0.845127	–3.856204	0.119285
12	C	–1.263825	–3.404744	1.414950
13	C	–3.399170	–2.646946	0.361395
14	C	–2.926405	–2.957918	–0.955133
15	C	–1.686672	–3.656109	–0.986710
16	H	–1.403021	–4.104387	–1.942868
17	O	–0.520721	–3.522570	2.503084
18	O	–3.567060	–2.629191	–2.063678
19	C	3.961887	–1.925764	0.154080
20	C	3.188178	–2.188414	1.323514
21	C	2.188728	–3.183129	1.148765
22	C	1.694315	–3.615497	–0.080736
23	C	2.320017	–3.145089	–1.275747
24	C	3.537806	–2.456197	–1.072710
25	H	1.687325	–3.586966	2.021996
26	H	4.168307	–2.256731	–1.936577
27	O	3.322204	–1.582259	2.500353
28	O	1.815363	–3.293763	–2.506745
29	C	3.166959	2.910636	0.136354
30	C	3.694145	2.346322	1.365443
31	C	4.501693	1.167693	1.225918
32	C	4.597938	0.433764	0.069211
33	C	4.015506	0.965528	–1.154542
34	C	3.353734	2.238746	–1.048588
35	H	4.985233	0.782530	2.121415
36	H	2.943753	2.666496	–1.958480
37	O	3.403915	2.804544	2.530885
38	O	4.075219	0.345731	–2.277411
39	C	–4.271599	1.707291	1.221223

40	C	–4.443822	0.310339	1.516745
41	C	–4.707178	–0.556037	0.383647
42	C	–4.701954	–0.012190	–0.879314
43	C	–4.212552	1.307832	–1.177574
44	C	–4.041224	2.194805	–0.042391
45	H	–4.152094	2.382191	2.061834
46	H	–4.916794	–0.679418	–1.708124
47	O	–4.287903	–0.120226	2.718984
48	O	–3.887293	1.624883	–2.381063
49	C	0.493115	–4.549011	–0.083346
50	H	0.636116	–5.282942	0.720731
51	H	0.466318	–5.096691	–1.031988
52	C	5.142318	–0.971860	0.134454
53	H	5.752261	–1.077827	1.037828
54	H	5.771401	–1.190982	–0.734571
55	C	2.358212	4.186700	0.197222
56	H	2.653867	4.840355	–0.628170
57	H	2.574248	4.689530	1.142421
58	C	–3.491461	3.591670	–0.221184
59	H	–3.779578	3.982670	–1.200085
60	H	–3.920075	4.243460	0.548473
61	C	–4.784882	–2.051280	0.555854
62	H	–5.470298	–2.469934	–0.189033
63	H	–5.155566	–2.296413	1.554868
64	C	–2.573001	–2.856919	1.469657
65	H	–2.950670	–2.569469	2.449636
66	Na	2.984423	0.499053	3.311944
67	Na	–0.191815	–2.302366	–2.598779
68	Na	0.883469	2.534443	–3.891033
69	Na	–2.309023	1.157580	3.258088
70	Na	0.851102	–1.854598	3.068054
71	Na	–2.957130	–0.590889	–2.925854
72	Na	2.673981	–1.157736	–3.210145

Table S9 Optimized geometry of $P5QNa_8$ (Single-point Energy = –3397.240956 Hartree, Gibbs Free Energy = –3397.405393 Hartree).

Serial number	Symbol	X	Y	Z
1	C	–0.989859	3.995993	0.562412
2	C	–2.335027	3.507043	0.550041
3	C	–2.842310	3.116435	–0.744861
4	C	–1.977502	3.064515	–1.831622
5	C	–0.598371	3.422847	–1.785152
6	C	–0.122345	3.957288	–0.523157
7	H	–0.658078	4.473415	1.485958
8	H	–2.370184	2.743035	–2.793924
9	O	–3.039700	3.438154	1.641704
10	O	0.161614	3.318015	–2.839138
11	C	–0.021341	–3.954712	0.532188
12	C	–0.500426	–3.410595	1.788113
13	C	–2.755591	–3.161482	0.755449
14	C	–2.248563	–3.560514	–0.535979
15	C	–0.896974	–4.031069	–0.546371
16	H	–0.567350	–4.529388	–1.460292
17	O	0.261206	–3.276821	2.838615
18	O	–2.958253	–3.512924	–1.627299
19	C	4.264046	–1.171754	0.198941
20	C	3.613950	–1.487145	1.431458
21	C	2.855522	–2.683885	1.401393
22	C	2.433646	–3.341730	0.241600
23	C	2.946486	–2.911815	–1.014580
24	C	3.979322	–1.947230	–0.927519
25	H	2.473048	–3.086076	2.333255
26	H	4.560841	–1.722881	–1.819239
27	O	3.649635	–0.750416	2.543488
28	O	2.497820	–3.317837	–2.209124
29	C	2.342290	3.390715	–0.249866
30	C	2.869474	2.962637	1.000552
31	C	3.926666	2.026152	0.900795
32	C	4.224616	1.265829	–0.231601
33	C	3.555024	1.570006	–1.456678
34	C	2.770309	2.748749	–1.416456
35	H	4.519408	1.810374	1.785888
36	H	2.373975	3.146481	–2.344493
37	O	2.419190	3.349778	2.200806
38	O	3.596822	0.837996	–2.570660
39	C	–4.606068	1.019903	0.884372

40	C	–4.388244	–0.296599	1.422793
41	C	–4.441701	–1.395608	0.467056
42	C	–4.559598	–1.103041	–0.871765
43	C	–4.383314	0.220358	–1.409153
44	C	–4.483996	1.316598	–0.454032
45	H	–4.700117	1.846939	1.579296
46	H	–4.618945	–1.934077	–1.565736
47	O	–4.120777	–0.456833	2.666730
48	O	–4.111877	0.387269	–2.651059
49	C	1.406336	–4.454154	0.383331
50	H	1.663538	–5.051908	1.267076
51	H	1.456410	–5.111033	–0.491459
52	C	5.121204	0.059890	–0.023508
53	H	5.772083	0.247552	0.838752
54	H	5.762662	–0.108270	–0.896661
55	C	1.294596	4.484456	–0.376727
56	H	1.535107	5.095188	–1.256163
57	H	1.335833	5.133392	0.504288
58	C	–4.305063	2.744879	–0.901598
59	H	–4.601875	2.856484	–1.947547
60	H	–4.923402	3.405086	–0.283706
61	C	–4.225017	–2.817884	0.917172
62	H	–4.831924	–3.493773	0.304860
63	H	–4.514531	–2.931608	1.964890
64	C	–1.885975	–3.079284	1.836904
65	H	–2.280184	–2.753922	2.797497
66	Na	3.112647	1.291056	3.302059
67	Na	0.374884	–2.682506	–2.510745
68	Na	1.317995	1.397554	–3.165883
69	Na	–2.756821	1.544713	2.948907
70	Na	1.406802	–1.357185	3.164155
71	Na	–2.707105	–1.610932	–2.931496
72	Na	3.054853	–1.217881	–3.258242
73	Na	0.337746	2.584199	2.469546

Table S10 Optimized geometry of $P5QNa_9$ (Single-point Energy = –3559.625174 Hartree, Gibbs Free Energy = –3559.802530 Hartree).

Serial number	Symbol	X	Y	Z
1	6	–0.933893	–4.252018	–0.544859
2	6	–2.209778	–3.652682	–0.716099
3	6	–2.843032	–3.273690	0.500756
4	6	–2.096588	–3.292333	1.684991
5	6	–0.704379	–3.538905	1.766493
6	6	–0.147722	–4.161443	0.607268
7	1	–0.502396	–4.779195	–1.395664
8	1	–2.621974	–3.017954	2.596479
9	8	–2.705700	–3.465670	–1.937177
10	8	–0.025928	–3.179488	2.859654
11	6	0.209070	4.167842	–0.630823
12	6	–0.344150	3.624883	–1.835357
13	6	–2.529788	3.429645	–0.639848
14	6	–1.996786	3.992397	0.558715
15	6	–0.628346	4.367611	0.485056
16	1	–0.228324	4.920052	1.340581
17	8	0.338354	3.475278	–2.960569
18	8	–2.719305	4.159001	1.656329
19	6	4.239817	1.007094	–0.516533
20	6	3.532269	1.380930	–1.695549
21	6	2.892958	2.641912	–1.617373
22	6	2.619269	3.342374	–0.437843
23	6	3.178680	2.865300	0.780377
24	6	4.103103	1.803917	0.627627
25	1	2.463687	3.075684	–2.513052
26	1	4.722270	1.530326	1.481290
27	8	3.418652	0.644375	–2.810247
28	8	2.864967	3.314854	2.005803
29	6	2.290183	–3.593467	0.227636
30	6	2.570891	–3.110994	–1.082403
31	6	3.638258	–2.179904	–1.135426
32	6	4.135485	–1.453317	–0.048763
33	6	3.679551	–1.785346	1.260255
34	6	2.919826	–2.981458	1.317398
35	1	4.074751	–1.939929	–2.102557
36	1	2.742030	–3.433128	2.292730
37	8	1.910408	–3.444565	–2.197476
38	8	3.882945	–1.067983	2.370912
39	6	–4.715540	–0.798554	–0.927842

40	6	–4.567410	0.570516	–1.359055
41	6	–4.144134	1.523214	–0.341554
42	6	–3.826840	1.059899	0.913409
43	6	–3.857330	–0.321365	1.302304
44	6	–4.317574	–1.273424	0.299494
45	1	–5.127868	–1.499762	–1.653486
46	1	–3.499919	1.781516	1.655353
47	8	–4.739997	0.886358	–2.585232
48	8	–3.497229	–0.680587	2.483768
49	6	1.683460	4.540949	–0.532041
50	1	1.964446	5.121654	–1.421634
51	1	1.828694	5.187077	0.341501
52	6	5.038246	–0.275204	–0.367153
53	1	5.585483	–0.496311	–1.291918
54	1	5.778065	–0.136229	0.430298
55	6	1.276466	–4.680562	0.528869
56	1	1.551114	–5.151923	1.480769
57	1	1.315011	–5.456673	–0.244996
58	6	–4.271367	–2.761593	0.560108
59	1	–4.685394	–2.982046	1.550467
60	1	–4.888557	–3.268833	–0.188441
61	6	–3.979871	2.986394	–0.686232
62	1	–4.544428	3.587010	0.034988
63	1	–4.395061	3.151434	–1.683872
64	6	–1.718492	3.271876	–1.765294
65	1	–2.166588	2.864126	–2.672507
66	11	2.377336	–1.320157	–3.230091
67	11	0.698470	3.077040	2.415957
68	11	1.702752	–1.774220	3.192197
69	11	–3.131101	–1.528806	–2.945853
70	11	1.276823	1.543964	–3.467682
71	11	–2.409881	3.201444	3.556212
72	11	3.130192	1.024922	2.863947
73	11	–0.271434	–2.969863	–2.639237
74	11	–1.394014	–1.193637	3.130305

Table S11 Optimized geometry of $P5QNa_{10}$ (Single-point Energy = –3721.998156 Hartree, Gibbs Free Energy = –3722.177739 Hartree)

Serial number	Symbol	X	Y	Z
1	C	–1.853262	–3.790459	–1.134602
2	C	–2.865564	–2.810909	–1.296824
3	C	–3.547599	–2.483079	–0.087824
4	C	–3.029173	–2.956884	1.122427
5	C	–1.777653	–3.601865	1.285549
6	C	–1.243938	–4.136737	0.076243
7	H	–1.456810	–4.276359	–2.025202
8	H	–3.623451	–2.747757	2.010761
9	O	–3.085407	–2.271139	–2.501318
10	O	–1.196744	–3.642529	2.489150
11	C	1.401404	4.082763	–0.084937
12	C	0.658032	3.951151	–1.294159
13	C	–1.434103	4.072254	0.076839
14	C	–0.689362	3.946976	1.286724
15	C	0.702542	4.157702	1.123976
16	H	1.305092	4.332234	2.013579
17	O	1.154520	3.645306	–2.498604
18	O	–1.181807	3.641911	2.491677
19	C	4.335297	–0.070878	–0.076296
20	C	3.987950	0.600764	–1.285399
21	C	3.741871	1.986367	–1.119241
22	C	3.443665	2.621040	0.090776
23	C	3.557417	1.873284	1.299208
24	C	4.188749	0.614522	1.134513
25	H	3.715371	2.615503	–2.006907
26	H	4.538480	0.091685	2.023165
27	O	3.865526	0.040910	–2.494036
28	O	3.109199	2.244791	2.504057
29	C	1.269883	–4.128223	–0.086672
30	C	1.802048	–3.584921	–1.292700
31	C	3.049070	–2.932121	–1.123417
32	C	3.561801	–2.460328	0.090094
33	C	2.881108	–2.799944	1.296171
34	C	1.874993	–3.784365	1.126917
35	H	3.644639	–2.713863	–2.008545
36	H	1.480246	–4.278567	2.013227
37	O	1.225618	–3.626752	–2.498367
38	O	3.097143	–2.263474	2.502610
39	C	–4.200733	0.585286	–1.127734

40	C	–3.577686	1.846851	–1.296844
41	C	–3.465015	2.597828	–0.090255
42	C	–3.751754	1.962479	1.122830
43	C	–3.986245	0.574587	1.290655
44	C	–4.337029	–0.099036	0.084569
45	H	–4.548264	0.056068	–2.012835
46	H	–3.720196	2.593046	2.010007
47	O	–3.131721	2.218727	–2.502976
48	O	–3.850283	0.014097	2.498290
49	C	2.916149	4.041851	0.002990
50	H	3.358859	4.521797	–0.878119
51	H	3.229096	4.616436	0.883212
52	C	4.755809	–1.526643	0.007202
53	H	5.345898	–1.800468	–0.875690
54	H	5.399081	–1.653037	0.886503
55	C	0.015739	–4.979499	–0.008074
56	H	0.094373	–5.630985	0.870782
57	H	–0.058734	–5.625522	–0.891156
58	C	–4.747590	–1.557879	0.001827
59	H	–5.333073	–1.835546	0.886490
60	H	–5.393316	–1.687967	–0.875113
61	C	–2.948025	4.022205	–0.007954
62	H	–3.392020	4.501604	0.872988
63	H	–3.266167	4.592789	–0.888898
64	C	–0.736233	4.150228	–1.133202
65	H	–1.340224	4.315250	–2.024806
66	Na	2.697229	–0.107884	3.105213
67	Na	0.944009	2.531504	3.122676
68	Na	–2.120693	1.654516	3.098334
69	Na	0.724389	–2.584404	3.094378
70	Na	–2.263470	–1.497527	3.101510
71	Na	2.289046	–1.476855	–3.109338
72	Na	2.120030	1.686169	–3.105589
73	Na	–0.706978	–2.566534	–3.087389
74	Na	–0.949182	2.484593	–3.090691
75	Na	–2.710983	–0.115152	–3.106156

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