Supporting Information

Electronic States of Quinones for Organic Energy Devices: The Effect of Molecular Structure on Electrochemical Characteristics

Naoka Nagamura[†,‡,‖], *Ryosuke Taniki*[‡], *Yuta Kitada*[‡], *Asuna Masuda*[‡], *Hiroaki Kobayashi*[‡], *Takashi Oka*[⊥], *and Itaru Honma*[‡,*]

† National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki, 305-0047, Japan
‡ Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1, Katahira, Aoba-ku, Sendai, 980-8577, Japan
‖ Japan Science and Technology Agency, PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama, 332-0012, Japan
⊥ Faculty of Humanity-Oriented Science and Engineering, Kindai University, 11-6, Kayanomori, Iizuka, Fukuoka, 820-8555, Japan

*E-mail: itaru.honma.e8@tohoku.ac.jp

I. Preparation process of cathode electrodes

Although spectroscopy measurements were performed using pristine powders, but electrochemical results were obtained using compounds as cathode electrodes. Here we present detail preparation process of cathode active materials containing quinones.

Quinone-dissolved acetone was stirred with acetylene black (AB; FX35, Denkikagaku Kogyo), kedjenblack (KB; EC600JD, Lion Specialty Chemicals Co., Ltd.), or activated carbon (AC; Maxsorb®, KNASAI COKE CHEMICALS COMPANY) for dispersion of carbon and adsorption of quinones, followed by removing acetone under a vacuum. Quinone-supported AC was mixed with polyethylene oxide (PEO, MW=4.0×10^6; Wako Pure Chemical Industries, Ltd) and lithium bis (trifluoromethylsulfonyl) amide (LiTFSA; KANTO CHEMICAL CO., INC) in water, followed by removing water at 60°C under a vacuum of 1 Pa. Electrodes were made by mixing obtained powder, AB, and polytetrafluoroethylene (PTFE; PTFE 6-J, Du Pont-Mitsui Fluorochemicals Co., Ltd.) and were pressed on SUS mesh in an Ar-filled globe box. Weight ratio of quinone, carbon, PEO, LiTFSA, AB, and PTFE was 20.8, 48.5, 11.5, 9.3, 5, and 5%. Electrolyte was a complex solution of LiTFSA

and tetraethyleneglycoldimethylether (G4; Sigma-Aldrich, >99%) at a ratio of 1:1 by mole. Prepared electrode, Li metal as a counter electrode, separator (Celgard® #2400, Celgard, LLC.), and electrolyte were fabricated in a CR2032 coin cell.

II. Cycle performance of composite electrodes with different kinds of support carbons

Figure S1 shows cycle performances of composite electrodes with different carbons; AB-NQ, AB-NQ-PEO, KB-NQ, KB-NQ-PEO, AC-NQ, AC-NQ-PEO. Composite electrode based on a carbon with a higher specific area gives a higher discharge capacity. Cycle performance of composite electrode with AC is improved by the wrapping of the polymer.

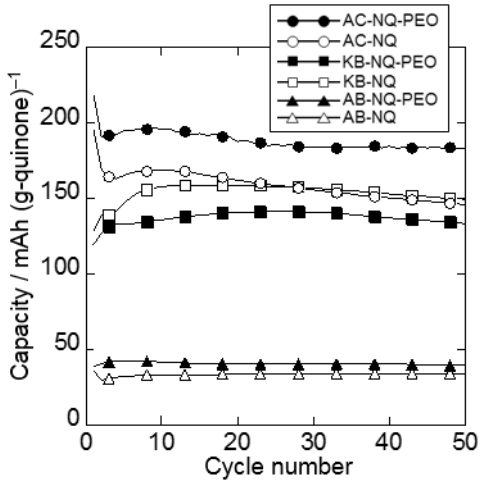

Figure S1. Cycle performances of composite electrodes with different carbons; AB-NQ, AB-NQ-PEO, KB-NQ, KB-NQ-PEO, AC-NQ, and AC-NQ-PEO.

III. Cycle and rate performance of composite electrodes based on different structures of quinones

Figure S2 (A) and (B) show charge-discharge curves of N2PQ at 0.2, 0.5, and 1.0 C and CVs at several scan rates of 0.02, 0.05, 0.1, and 0.2 mV s^{-1}. Two plateaus and peaks appear in charge-discharge and CV tests, respectively. Discharge capacities in the 5th cycle at 0.2 and 1.0 C are 229, 219, and 194 mAh g^{-1}, respectively, and the utilization ratios of N2PQ (theoretical discharge capacity: 255 mAh g^{-1}) are 89, 85, and 76 %. When charge/discharge rates become high, two peaks at the cathodic scan in CVs become broad and two plateaus in galvanostatic tests become polarized. In the reduction process of N2PQ, one electron is accepted from the current collector and subsequently one

lithium ion is coordinated from electrolyte to the reduced quinone. An overpotential behavior of this reduction is caused by these two steps, acceptance of electron and coordination of lithium ion. The former should also affect the oxidation reaction and there appears a little overpotential behavior in oxidation. Thus the increase of the overpotential in reduction process of N2PQ is plausibly caused by a coordination of lithium ion from electrolytes to quinones.

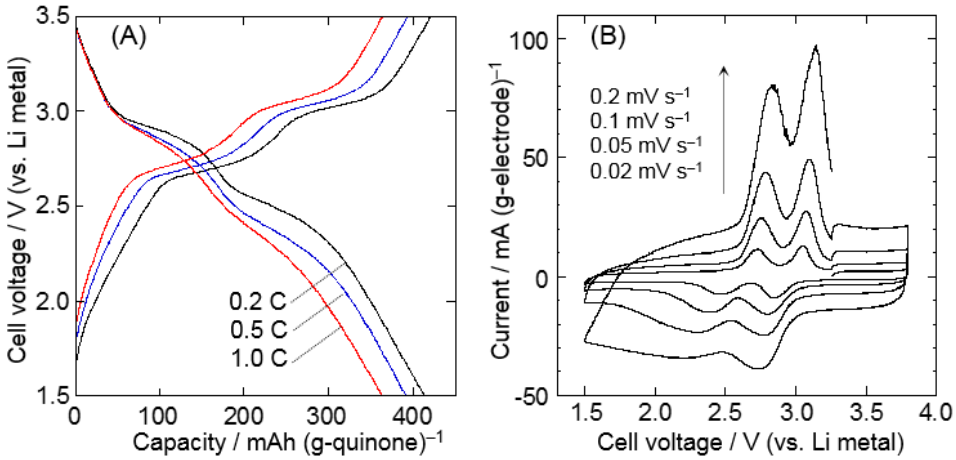

Figure S2. (A) Charge-discharge curves of N2PQ at 0.2, 0.5, and 1.0 C and (B) CVs at several scan rates of 0.02, 0.05, 0.1, and 0.2 mV s^{-1}.

Figure S3 shows cycle performance of composite electrodes. Capacities decrease to a certain level during cycles because the dissolution of quinones is large for preventing by covering polymer.

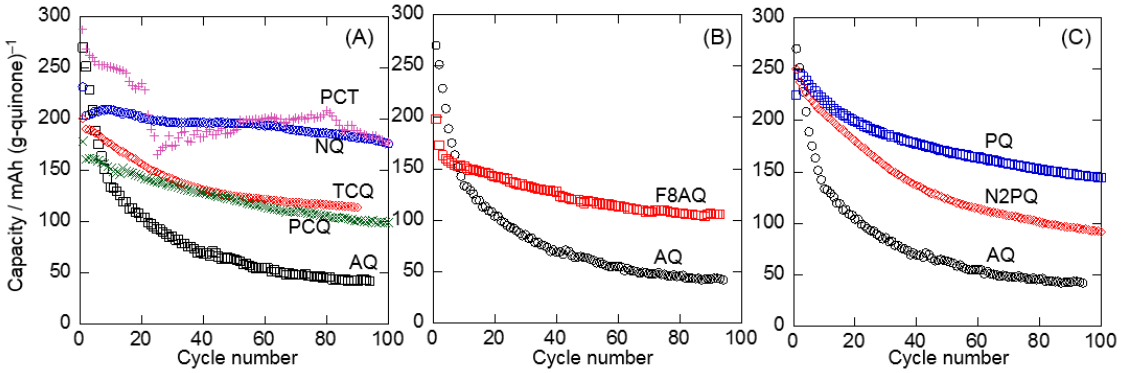

Figure S3. The cycle performances of electrodes based on (A) NQ, AQ, TCQ, PCQ, PCT, (B) F8AQ, (C) PQ, and N2PQ.

IV. Computational Methods

All calculations were performed using the Gaussian 09. The initial geometries of the quinone derivatives in neutral states (states 1), excited states (state 2), reduced states (states 3), and lithiated states (states 4) were generated with GaussView[R1]. Optimized geometries are computed in redundant internal coordinates at the wB97XD level of theory and the 6-311++G(d,p) basis set either with or without Li chemisorption.

$\Delta G_{1\to2}$, $\Delta G_{2\to3}$, and $\Delta G_{3\to4}$ mentioned in Table 2 in the manuscript are obtained using;

$$\Delta G_{1\to2} = \left(E^{\mathrm{Q}}_{\mathrm{LUMO}} + E^{\mathrm{Li+}}_{0} - E^{\mathrm{Li}}_{0}\right) \times 2$$

$$\Delta G_{2\to3} = E^{\mathrm{Q-}}_{0} + 2 \times E^{\mathrm{Li+}}_{0} - E^{\mathrm{Q}}_{0} - 2 \times E^{\mathrm{Li}}_{0} - \Delta G_{1\to2}$$

$$\Delta G_{3\to4} = E^{\mathrm{QLi}}_{0} - E^{\mathrm{Q-}}_{0} - 2 \times E^{\mathrm{Li+}}_{0}$$

where $E^{\mathrm{Q}}_{\mathrm{LUMO}}$ is the LUMO energy of neutral quinones. Here $E^{\mathrm{Q}}_{0}, E^{\mathrm{Q-}}_{0}, E^{\mathrm{QLi}}_{0}, E^{\mathrm{Li}}_{0}$, and $E^{\mathrm{Li+}}_{0}$ are the total electronic energy corrected for the zero-point energy of the bare (neutral) quinone derivative, the quinone anion (state 3), the lithiated quinone derivative, the Li atom, and the Li ion, respectively.

Optimized structures of quinones in neutral states (states 1), anions (states 3), and lithiated states (states 4) are presented in the Cartesian coordinate notation in Table S1-S20. Molecular orbital energies in the optimized structures are obtained and compared among molecular structures.

Table S1. Calculated cartesian coordinates (Å) of the optimized geometry of AQ in a neutral state (state1).

Atom	X	Y	Z	Atom	X	Y	Z
C1	3.68289	0.69661	0.00039	C13	-3.68289	-0.69661	0.00038
C2	2.48389	1.39234	0.00015	C14	-2.48389	-1.39234	0.00013
C3	1.27506	0.69991	-0.00005	H1	-2.46038	2.47553	0.00015
C4	1.27506	-0.69991	-0.00006	H2	4.62199	1.23814	0.00058
C5	2.48389	-1.39234	0.00014	H3	2.46038	2.47553	0.00013
C6	3.68289	-0.69661	0.00038	H4	2.46038	-2.47553	0.00011
C7	0.00000	1.47534	-0.00026	H5	4.62199	-1.23813	0.00057
C8	0.00000	-1.47534	-0.00027	H6	-4.62199	1.23813	0.00058
C9	-1.27506	-0.69991	-0.00006	H7	-4.62199	-1.23813	0.00056
C10	-1.27506	0.69991	-0.00005	H8	-2.46038	-2.47553	0.00010
C11	-2.48389	1.39234	0.00016	O1	0.00000	-2.68768	-0.00067
C12	-3.68289	0.69661	0.00039	O2	0.00000	2.68768	-0.00071

Table S2. Calculated cartesian coordinates (Å) of the optimized geometry of TCQ in a neutral state (state1).

Atom	X	Y	Z	Atom	X	Y	Z
C1	2.37143	0.70025	-0.00007	C16	3.58151	1.39180	0.00017
C2	1.09949	1.48227	-0.00030	C17	4.78035	0.69675	0.00038
C3	-0.17580	0.71164	-0.00018	C18	4.78035	-0.69682	0.00018
C4	-0.17577	-0.71161	-0.00015	H1	-3.83600	2.48482	0.00013
C5	1.09954	-1.48223	-0.00018	H2	-1.34164	2.48022	-0.00013
C6	-1.36398	1.39569	-0.00009	H3	-1.34159	-2.48021	-0.00008
C7	-1.36395	-1.39568	-0.00007	H4	-5.96340	1.24055	0.00030
C8	-2.60081	-0.71089	0.00002	H5	-5.96338	-1.24063	0.00029
C9	-2.60083	0.71088	0.00002	H6	-3.83595	-2.48486	0.00012
C10	-3.83997	1.40003	0.00012	H7	3.55715	2.47494	0.00021
C11	-5.01971	0.70711	0.00022	H8	3.55705	-2.47493	0.00029
C12	-5.01969	-0.70717	0.00021	H9	5.71922	1.23868	0.00071
C13	-3.83994	-1.40007	0.00012	H10	5.71932	-1.23858	0.00048
C14	2.37145	-0.70018	-0.00001	O1	1.10858	2.69542	-0.00034
C15	3.58149	-1.39178	0.00018	O2	1.10870	-2.69538	-0.00037

Table S3. Calculated cartesian coordinates (Å) of the optimized geometry of PCQ in a neutral state (state1).

Atom	X	Y	Z	Atom	X	Y	Z
C1	1.27254	0.71191	-0.00056	C19	4.93782	-1.40013	0.00064
C2	-0.00001	1.48897	-0.00091	C20	6.11738	-0.70730	0.00107
C3	-1.27254	0.71191	-0.00057	C21	6.11738	0.70729	0.00106
C4	-1.27254	-0.71190	-0.00057	C22	4.93782	1.40013	0.00061
C5	0.00000	-1.48896	-0.00094	H1	-4.93373	2.48494	0.00065
C6	-2.46182	1.39506	-0.00022	H2	-2.43884	2.47957	-0.00028
C7	-2.46181	-1.39506	-0.00023	H3	-2.43883	-2.47956	-0.00029
C8	-3.69840	-0.71090	0.00020	H4	-7.06112	1.24066	0.00142
C9	-3.69840	0.71090	0.00020	H5	-7.06112	-1.24067	0.00141
C10	-4.93782	1.40014	0.00065	H6	-4.93373	-2.48494	0.00064
C11	-6.11737	0.70728	0.00107	H7	2.43887	2.47956	-0.00029
C12	-6.11737	-0.70729	0.00107	H8	7.06114	-1.24065	0.00144
C13	-4.93781	-1.40014	0.00064	H9	7.06113	1.24067	0.00141
C14	1.27253	-0.71191	-0.00055	H10	4.93371	2.48493	0.00061

C15	2.46181	-1.39506	-0.00019	H11	4.93372	-2.48493	0.00067
C16	3.69840	-0.71091	0.00022	H12	2.43882	-2.47957	-0.00026
C17	3.69839	0.71089	0.00020	O1	0.00001	2.70282	-0.00143
C18	2.46181	1.39506	-0.00021	O2	-0.00001	-2.70282	-0.00145

Table S4. Calculated cartesian coordinates (Å) of the optimized geometry of F8AQ in a neutral state (state1).

Atom	X	Y	Z	Atom	X	Y	Z
C1	0.00000	2.45387	1.39190	C13	0.00000	0.00000	1.49020
C2	0.00000	3.62643	0.70987	C14	0.00000	1.20381	0.69669
C3	0.00000	3.62643	-0.70987	F1	0.00000	2.46265	2.71383
C4	0.00000	2.45387	-1.39190	F2	0.00000	4.78891	1.34331
C5	0.00000	1.20381	-0.69669	F3	0.00000	4.78891	-1.34331
C6	0.00000	0.00000	-1.49020	F4	0.00000	2.46265	-2.71383
C7	0.00000	-1.20381	-0.69669	F5	0.00000	-2.46265	-2.71383
C8	0.00000	-2.45387	-1.39190	F6	0.00000	-4.78891	-1.34331
C9	0.00000	-3.62643	-0.70987	F7	0.00000	-4.78891	1.34331
C10	0.00000	-3.62643	0.70987	F8	0.00000	-2.46265	2.71383
C11	0.00000	-2.45387	1.39190	O1	0.00000	0.00000	-2.74048
C12	0.00000	-1.20381	0.69669	O2	0.00000	0.00000	2.74048

Table S5. Calculated cartesian coordinates (Å) of the optimized geometry of PQ in a neutral state (state1).

Atom	X	Y	Z	Atom	X	Y	Z
C1	0.00000	0.74366	-0.77890	C13	0.00000	3.56533	-0.75733
C2	0.00000	-0.74366	-0.77890	C14	0.00000	-3.56533	-0.75733
C3	0.00000	1.46341	0.42877	H1	0.00000	0.97501	-2.92575
C4	0.00000	1.47858	-1.96845	H2	0.00000	-0.97501	-2.92575
C5	0.00000	-1.46341	0.42877	H3	0.00000	3.36671	1.38876
C6	0.00000	-1.47858	-1.95916	H4	0.00000	3.40220	-2.90107
C7	0.00000	0.77274	1.74301	H5	0.00000	-3.36671	1.38876
C8	0.00000	2.85880	0.43160	H6	0.00000	-3.40220	-2.90107
C9	0.00000	2.86517	-1.95916	H7	0.00000	4.64887	-0.75200
C10	0.00000	-0.77274	1.74301	H8	0.00000	-4.64887	-0.75200
C11	0.00000	-2.85880	0.43160	O1	0.00000	1.36005	2.79411
C12	0.00000	-2.86517	-1.95916	O2	0.00000	-1.36005	2.79411

Table S6. Calculated cartesian coordinates (Å) of the optimized geometry of N2PQ in a neutral state (state1).

Atom	X	Y	Z	Atom	X	Y	Z
C1	0.00000	0.74686	-0.77581	C12	0.00000	-3.48243	-0.83595
C2	0.00000	-0.74686	-0.77581	N1	0.00000	1.35835	-1.95871
C3	0.00000	1.45785	0.43266	N2	0.00000	-1.35835	-1.95871
C4	0.00000	-1.45785	0.43266	H1	0.00000	3.40252	1.32552
C5	0.00000	0.77408	1.74927	H2	0.00000	3.14250	-2.96445
C6	0.00000	2.85115	0.39224	H3	0.00000	-3.40252	1.32552
C7	0.00000	2.68527	-1.97880	H4	0.00000	-3.14250	-2.96445
C8	0.00000	-0.77408	1.74927	H5	0.00000	4.56211	-0.91925
C9	0.00000	-2.85115	0.39224	H6	0.00000	-4.56211	-0.91925
C10	0.00000	-2.68527	-1.97880	O1	0.00000	1.36764	2.79594
C11	0.00000	3.48243	-0.83595	O2	0.00000	-1.36764	2.79594

Table S7. Calculated cartesian coordinates (Å) of the optimized geometry of AQ anion (state3).

Atom	X	Y	Z	Atom	X	Y	Z
C1	3.64975	0.71277	0.00221	C13	-3.64987	-0.71285	0.00150
C2	2.47336	1.40435	-0.00262	C14	-2.47338	-1.40435	-0.00105
C3	1.21758	0.71438	-0.00191	H1	-2.45965	2.50479	0.00406
C4	1.21747	-0.71440	-0.00158	H2	4.61562	1.23916	0.00409
C5	2.47318	-1.40448	0.00207	H3	2.45983	2.50472	-0.00404
C6	3.64965	-0.71304	0.00460	H4	2.45945	-2.50485	0.00195
C7	0.00003	1.40362	-0.00190	H5	4.61573	-1.23903	0.00696
C8	-0.00011	-1.40356	-0.00253	H6	-4.61576	1.23914	0.00620
C9	-1.21769	-0.71429	-0.00179	H7	-4.61587	-1.23904	0.00312
C10	-1.21759	0.71444	-0.00022	H8	-2.45959	-2.50474	-0.00279
C11	-2.47332	1.40440	0.00194	O1	0.00041	2.83362	-0.00215
C12	-3.64979	0.71290	0.00383	O2	0.00017	-2.83356	-0.00222

Table S8. Calculated cartesian coordinates (Å) of the optimized geometry of TCQ anion (state3).

Atom	X	Y	Z	Atom	X	Y	Z
C1	2.30070	0.72465	-0.00035	C16	3.55891	1.39038	0.00023
C2	1.10303	1.51166	-0.00091	C17	4.74954	0.71444	0.00076
C3	-0.11370	0.73049	-0.00060	C18	4.74954	-0.71444	0.00077
C4	-0.11370	-0.73049	-0.00059	H1	-3.82150	2.48678	0.00026
C5	1.10303	-1.51166	-0.00088	H2	-1.31168	2.48094	-0.00032
C6	-1.34705	1.39396	-0.00030	H3	-1.31168	-2.48094	-0.00030
C7	-1.34705	-1.39396	-0.00029	H4	-5.95445	1.25511	0.00076
C8	-2.56560	-0.72452	-0.00002	H5	-5.95445	-1.25511	0.00076
C9	-2.56560	0.72452	-0.00002	H6	-3.82150	-2.48678	0.00027
C10	-3.82670	1.39848	0.00026	H7	3.52179	2.47633	0.00019
C11	-5.00961	0.71711	0.00054	H8	3.52179	-2.47633	0.00023
C12	-5.00961	-0.71711	0.00055	H9	5.69234	1.25925	0.00118
C13	-3.82670	-1.39848	0.00027	H10	5.69234	-1.25926	0.00119
C14	2.30070	-0.72465	-0.00034	O1	1.09704	2.79449	0.00004
C15	3.55892	-1.39038	0.00024	O2	1.09704	-2.79449	-0.00007

Table S9. Calculated cartesian coordinates (Å) of the optimized geometry of PCQ anion (state3).

Atom	X	Y	Z	Atom	X	Y	Z
C1	-1.21030	0.73067	0.00016	C19	-4.92427	-1.39957	0.00008
C2	-0.00002	1.51406	0.00022	C20	-6.10548	-0.71782	-0.00007
C3	1.21031	0.73065	0.00006	C21	-6.10549	0.71778	-0.00025
C4	1.21030	-0.73067	0.00000	C22	-4.92430	1.39955	-0.00021
C5	0.00001	-1.51406	0.00006	H1	4.91917	2.48768	-0.00031
C6	2.44605	1.39443	-0.00004	H2	2.41228	2.48119	-0.00010
C7	2.44607	-1.39444	-0.00003	H3	2.41229	-2.48120	0.00004
C8	3.66211	-0.72497	-0.00007	H4	7.05067	1.25483	-0.00035
C9	3.66210	0.72496	-0.00012	H5	7.05068	-1.25476	0.00033
C10	4.92427	1.39957	-0.00020	H6	4.91921	-2.48766	0.00029
C11	6.10548	0.71783	-0.00014	H7	-2.41230	2.48120	0.00003
C12	6.10549	-0.71778	0.00004	H8	-7.05067	-1.25482	0.00006
C13	4.92431	-1.39955	0.00010	H9	-7.05068	1.25476	-0.00061
C14	-1.21030	-0.73066	0.00011	H10	-4.91921	2.48766	-0.00040

C15	-2.44605	-1.39444	0.00011	H11	-4.91917	-2.48768	0.00019
C16	-3.66210	-0.72496	0.00010	H12	-2.41228	-2.48119	0.00016
C17	-3.66211	0.72497	0.00004	O1	-0.00006	2.79283	0.00027
C18	-2.44607	1.39444	0.00009	O2	0.00007	-2.79283	-0.00021

Table S10. Calculated cartesian coordinates (Å) of the optimized geometry of F8AQ anion (state3).

Atom	X	Y	Z	Atom	X	Y	Z
C1	0.00000	2.48436	1.38596	C13	0.00000	0.00000	1.51372
C2	0.00000	3.66319	0.70405	C14	0.00000	1.21568	0.72862
C3	0.00000	3.66319	-0.70405	F1	0.00000	2.60923	2.72420
C4	0.00000	2.48436	-1.38596	F2	0.00000	4.85629	1.35280
C5	0.00000	1.21568	-0.72862	F3	0.00000	4.85629	-1.35280
C6	0.00000	0.00000	-1.51372	F4	0.00000	2.60923	-2.72420
C7	0.00000	-1.21568	-0.72862	F5	0.00000	-2.60923	-2.72420
C8	0.00000	-2.48436	-1.38596	F6	0.00000	-4.85629	-1.35280
C9	0.00000	-3.66319	-0.70405	F7	0.00000	-4.85629	1.35280
C10	0.00000	-3.66319	0.70405	F8	0.00000	-2.60923	2.72420
C11	0.00000	-2.48436	1.38596	O1	0.00000	0.00000	-2.78110
C12	0.00000	-1.21568	0.72862	O2	0.00000	0.00000	2.78110

Table S11. Calculated cartesian coordinates (Å) of the optimized geometry of PQ anion (state3).

Atom	X	Y	Z	Atom	X	Y	Z
C1	0.00000	0.71212	-0.82395	C13	0.00000	3.54783	-0.72469
C2	0.00000	-0.71212	-0.82395	C14	0.00000	-3.54783	-0.72469
C3	0.00000	1.39091	0.45003	H1	0.00000	1.00400	-2.96950
C4	0.00000	1.50054	-2.00217	H2	0.00000	-1.00400	-2.96950
C5	0.00000	-1.39091	0.45003	H3	0.00000	3.29507	1.40882
C6	0.00000	-1.50054	-2.00217	H4	0.00000	3.43992	-2.90976
C7	0.00000	0.73418	1.74521	H5	0.00000	-3.29507	1.40882
C8	0.00000	2.81529	0.43448	H6	0.00000	-3.43992	-2.90976
C9	0.00000	2.87650	-1.97841	H7	0.00000	4.63647	-0.68777
C10	0.00000	-0.73418	1.74521	H8	0.00000	-4.63647	-0.68777
C11	0.00000	-2.81529	0.43448	O1	0.00000	1.41159	2.81941
C12	0.00000	-2.87650	-1.97841	O2	0.00000	-1.41159	2.81941

Table S12. Calculated cartesian coordinates (Å) of the optimized geometry of N2PQ anion (state3).

Atom	X	Y	Z	Atom	X	Y	Z
C1	0.00000	0.70958	-0.83894	C12	0.00000	-3.47147	-0.78321
C2	0.00000	-0.70958	-0.83894	N1	0.00000	1.40095	-2.01285
C3	0.00000	1.37786	0.44551	N2	0.00000	-1.40095	-2.01285
C4	0.00000	-1.37786	0.44551	H1	0.00000	3.29943	1.36969
C5	0.00000	0.73286	1.74673	H2	0.00000	3.22082	-2.94933
C6	0.00000	2.79324	0.40840	H3	0.00000	-3.29943	1.36969
C7	0.00000	2.71107	-1.98172	H4	0.00000	-3.22082	-2.94933
C8	0.00000	-0.73286	1.74673	H5	0.00000	4.55917	-0.82436
C9	0.00000	-2.79324	0.40840	H6	0.00000	-4.55917	-0.82436
C10	0.00000	-2.71107	-1.98172	O1	0.00000	1.42081	2.81417
C11	0.00000	3.47147	-0.78321	O2	0.00000	-1.42081	2.81417

Table S13. Calculated cartesian coordinates (Å) of the optimized geometry of Li_2AQ (state4).

Atom	X	Y	Z	Atom	X	Y	Z
C1	-3.64812	0.70453	0.09819	C14	2.46876	-1.38549	-0.18044
C2	-2.46869	1.38546	0.18051	H1	2.44894	2.45631	0.35116
C3	-1.21337	0.71275	0.07879	H2	-4.59125	1.23319	0.18777
C4	-1.21336	-0.71276	-0.07880	H3	-2.44888	2.45628	0.35131
C5	-2.46868	-1.38549	-0.18050	H4	-2.44886	-2.45631	-0.35130
C6	-3.64811	-0.70457	-0.09816	H5	-4.59124	-1.23323	-0.18773
C7	0.00004	1.44929	0.15729	H6	4.59132	1.23321	0.18769
C8	0.00004	-1.44930	-0.15732	H7	4.59132	-1.23322	-0.18765
C9	1.21345	-0.71275	-0.07878	H8	2.44894	-2.45632	-0.35116
C10	1.21345	0.71275	0.07877	O1	0.00002	2.77032	0.21844
C11	2.46876	1.38548	0.18044	O2	0.00003	-2.77034	-0.21846
C12	3.64819	0.70455	0.09815	Li1	-0.00070	2.84049	-1.51410
C13	3.64819	-0.70456	-0.09813	Li2	-0.00062	-2.84023	1.51412

Table S14. Calculated cartesian coordinates (Å) of the optimized geometry of Li_2TCQ (state4).

Atom	X	Y	Z	Atom	X	Y	Z
C1	2.20011	-0.72440	-0.07874	C17	4.65503	-0.69678	-0.17175
C2	1.00373	-1.46487	-0.08910	C18	4.65503	0.69682	0.17117
C3	-0.23388	-0.71616	-0.03551	H1	-3.91799	-2.48303	-0.14752
C4	-0.23386	0.71611	0.03586	H2	-1.42544	-2.47743	-0.13597
C5	1.00375	1.46476	0.08949	H3	-1.42544	2.47738	0.13624
C6	-1.45006	-1.39489	-0.07255	H4	-6.04077	-1.24220	-0.07602
C7	-1.45006	1.39484	0.07277	H5	-6.04077	1.24217	0.07549
C8	-2.66728	0.71544	0.03954	H6	-3.91800	2.48299	0.14735
C9	-2.66729	-0.71549	-0.03952	H7	3.47052	-2.40955	-0.59477
C10	-3.92199	-1.39959	-0.08170	H8	3.47064	2.40959	0.59440
C11	-5.09550	-0.71167	-0.04259	H9	5.59464	-1.20591	-0.35501
C12	-5.09550	0.71163	0.04221	H10	5.59468	1.20601	0.35410
C13	-3.92199	1.39955	0.08152	O1	1.00696	-2.77540	-0.07519
C14	2.20009	0.72440	0.07884	O2	1.00699	2.77543	0.07573
C15	3.47538	1.36560	0.28303	Li1	2.15732	-2.71018	1.26598
C16	3.47533	-1.36558	-0.28330	Li2	2.15604	2.71064	-1.26617

Table S15. Calculated cartesian coordinates (Å) of the optimized geometry of Li_2PCQ (state4).

Atom	X	Y	Z	Atom	X	Y	Z
C1	1.21690	-0.71591	-0.04483	C20	6.08877	0.77727	0.07200
C2	0.00192	-1.46730	-0.05392	C21	6.10506	-0.64180	-0.12070
C3	-1.21226	-0.72848	-0.04436	C22	4.94621	-1.34400	-0.19914
C4	-1.21687	0.71582	0.04490	H1	-4.88863	-2.51838	-0.30135
C5	-0.00183	1.46713	0.05387	H2	-2.40724	-2.48708	-0.20065
C6	-2.44124	-1.40589	-0.11391	H3	-2.48538	2.43344	0.39238
C7	-2.47194	1.37068	0.14816	H4	-7.02806	-1.31470	-0.13716
C8	-3.67532	0.68693	0.08346	H5	-7.05755	1.15273	0.20800
C9	-3.65786	-0.74544	-0.07931	H6	-4.96313	2.41904	0.35138
C10	-4.90890	-1.44182	-0.16465	H7	2.48511	-2.43371	-0.39191
C11	-6.08872	-0.77741	-0.07217	H8	7.02812	1.31454	0.13693
C12	-6.10502	0.64159	0.12071	H9	7.05761	-1.15293	-0.20791
C13	-4.94614	1.34378	0.19924	H10	4.96315	-2.41927	-0.35115

C14	1.21224	0.72841	0.04437	H11	4.88871	2.51827	0.30093
C15	2.44135	1.40580	0.11376	H12	2.40739	2.48700	0.20041
C16	3.65788	0.74532	0.07915	O1	0.02491	-2.77940	0.00136
C17	3.67534	-0.68713	-0.08346	O2	-0.02490	2.77926	-0.00147
C18	2.47203	-1.37086	-0.14811	Li1	-1.18792	2.75140	-1.33503
C19	4.90898	1.44169	0.16438	Li2	1.18672	-2.74743	1.33652

Table S16. Calculated cartesian coordinates (Å) of the optimized geometry of Li_2F8AQ (state4).

Atom	X	Y	Z	Atom	X	Y	Z
C1	2.44393	1.36476	0.00007	C14	1.16565	0.72681	-0.00006
C2	3.62722	0.70766	0.00009	F1	2.57242	2.73495	0.00028
C3	3.62722	0.70764	0.00004	F2	4.79337	1.35446	0.00026
C4	2.44394	1.36476	-0.00001	F3	4.79338	-1.35445	0.00012
C5	1.16566	-0.72681	-0.00008	F4	2.57244	-2.73493	0.00008
C6	-0.04307	-1.46357	-0.00025	F5	-2.62325	-2.71934	0.00024
C7	-1.26285	-0.71798	-0.00008	F6	-4.86780	-1.34310	0.00029
C8	-2.52241	-1.38933	0.00007	F7	-4.86782	1.34308	0.00014
C9	-3.69821	-0.70292	0.00012	F8	-2.62327	2.71933	-0.00002
C10	-3.69821	0.70290	0.00005	O1	-0.05566	-2.75977	-0.00055
C11	-2.52243	1.38933	-0.00004	O2	-0.05569	2.75979	-0.00055
C12	-1.26286	0.71798	-0.00012	Li1	1.10375	-3.99034	-0.00025
C13	-0.04308	1.46357	-0.00025	Li2	1.10372	3.99034	-0.00009

Table S17. Calculated cartesian coordinates (Å) of the optimized geometry of Li_2PQ (state4).

Atom	X	Y	Z	Atom	X	Y	Z
C1	-0.72880	-0.98642	0.00002	C14	3.54843	-0.90980	-0.00002
C2	0.72886	-0.98637	0.00001	H1	-0.99975	-3.13324	0.00065
C3	-1.42382	0.24666	-0.00020	H2	0.99994	-3.13317	-0.00062
C4	-1.49429	-2.16980	0.00033	H3	-3.32584	1.22853	-0.00047
C5	1.42382	0.24674	0.00023	H4	-3.43050	-3.06715	0.00061
C6	1.49443	-2.16971	-0.00031	H5	3.32581	1.22870	0.00050
C7	-0.69530	1.48961	-0.00025	H6	3.43069	-3.06696	-0.00060
C8	-2.83229	0.26407	-0.00025	H7	-4.63282	-0.88775	0.00002
C9	-2.87135	-2.13797	0.00033	H8	4.63290	-0.88750	-0.00003

C10	0.69526	1.48971	0.00031	O1	-1.31917	2.69126	-0.00054
C11	2.83229	0.26422	0.00027	O2	1.31897	2.69128	0.00058
C12	2.87149	-2.13781	-0.00032	Li1	-0.00108	3.18373	1.25260
C13	-3.54835	-0.90999	0.00002	Li2	0.00069	3.18275	-1.25307

Table S18. Calculated cartesian coordinates (Å) of the optimized geometry of Li_2N2PQ (state4).

Atom	X	Y	Z	Atom	X	Y	Z
C1	0.72990	-0.98871	-0.00073	N1	1.37952	-2.16678	0.00003
C2	-0.72997	-0.98865	-0.00072	N2	-1.37970	-2.16669	-0.00003
C3	1.41612	0.24785	-0.00122	H1	3.35380	1.17082	-0.00150
C4	-1.41610	0.24795	-0.00113	H2	3.18295	-3.12818	0.00087
C5	0.69503	1.49413	-0.00214	H3	-3.35375	1.17102	-0.00142
C6	2.82128	0.22686	-0.00096	H4	-3.18320	-3.12796	0.00087
C7	2.69587	-2.15588	0.00035	H5	4.55145	-1.04701	0.00000
C8	-0.69494	1.49424	-0.00188	H6	-4.55154	-1.04670	0.00007
C9	-2.82127	0.22704	-0.00092	O1	1.32236	2.69248	-0.00027
C10	-2.69605	-2.15570	0.00022	O2	-1.32189	2.69235	-0.00017
C11	3.46934	-0.98408	-0.00017	Li1	-0.00038	3.21461	-1.24379
C12	-3.46943	-0.98385	-0.00017	Li2	0.00003	3.17756	1.26430

Reference

(1) Dennington, R.; Keith, T.; Millam, J. *GaussView, Version 5*; Semichem Inc.: Shawnee Mission KS, **2009**.