Supporting Information

Cation Recognition on a Fullerene-Based Macrocycle

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Contents

1. General

The ^{1}H and ^{13}C NMR measurements were carried out at room temperature (unless otherwise noted) with JEOL JNM ECA500 and Bruker Avance III 800US Plus instruments. The NMR chemical shifts were reported in ppm with reference to residual protons and carbons of ODCB-d_4 (δ 7.20 ppm in ^{1}H NMR, δ 132.35 ppm in ^{13}C NMR). The ^{7}Li NMR chemical shifts were reported in ppm with reference to the chemical shift of LiCl (δ 0.00 ppm) in a sealed glass capillary inserted inside the NMR tube containing D_2O. The titration data was fitted using DynaFit.[1] APCI (atmospheric-pressure chemical ionization) and ESI (electrospray ionization) mass spectra were measured on a Bruker micrOTOF-Q II. UV-vis absorption spectra were measured with a Shimadzu UV-3150 spectrometer. Thin layer chromatography (TLC) was performed on glass plates coated with 0.25 mm thick silica gel 60F-254 (Merck). Column chromatography was performed using PSQ 60B or PSQ 100B (Fuji Silysia).

ODCB (*o*-dichlorobenzene), lithium tetraphenylborate tris(1,2-dimethoxyethane), potassium tetraphenylboratem, rubidium tetraphenylborate, and cesium tetraphenylborate were purchased from Sigma-Aldrich Co. LLC. Lithium tetrakis(pentafluorophenyl)borate - ethyl ether complex and sodium tetraphenylborate were purchased from Tokyo Chemical Industry Co. Ltd. Carbon disulfide and acetone were purchased from FUJIFILM Wako Pure Chemical Corporation. Distilled water was used for the reaction. Compounds **1** and H_2O@**1** were synthesized according to a literature.[2]

Unless otherwise noted, materials purchased from commercial suppliers were used without further purification.

2. Computational Methods

All calculations for the geometry optimization were conducted with Gaussian 09 program packages. The structures were optimized at the M06-2X/6-31G(d,p) level of theory without any symmetry assumptions. All structures at the stationary states were confirmed by the frequency analyses at the same level of theory. The single point calculations for drawing electrostatic potential maps were performed at the MP2/6-31G(d,p) level of theory using geometries optimized at the M06-2X/6-31G(d,p) level of theory. Using geometries optimized at the B3LYP/6-31G(d) level of theory, TD DFT calculations were carried out at the CAM-B3LYP/6-31G(d) level of theory.

3. Titration of 1 with a Lithium Salt

The titration using ^{7}Li and ^{1}H NMR was carried out by adding one portion of **1** (ca. 390 μg, ca. 0.35 μmol, ca. 0.20 equiv) to a solution of $Li^{+}[B(C_6F_5)_4]^{-}$•2.5Et_2O (1.50 mg, 1.72 μmol) in ODCB (0.600 mL) (Figure S1a, Table S1). During the titration, the solution color changed from reddish brown to dark black (Figure S1b).

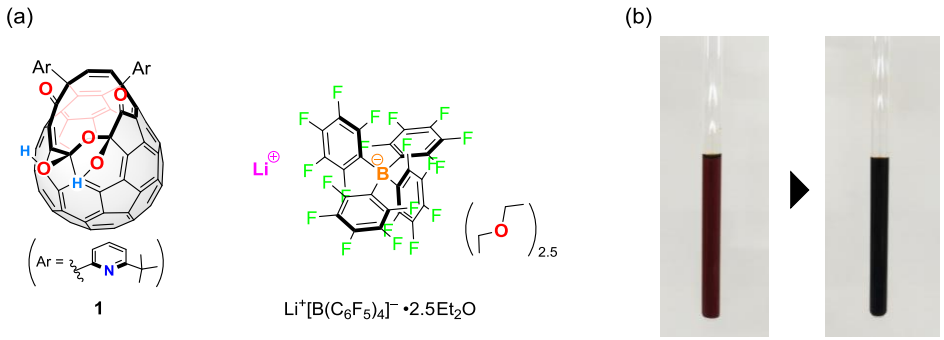


Figure S1. (a) Chemical structures of **1** and $Li^{+}[B(C_6F_5)_4]^{-}$•2.5Et_2O. (b) The solution color before and after titration.

Table S1. Titration results

Addition amount of **1** (μg)	Total amount of **1** (μmol)	(equiv)	(mM)	Molar ratio $x(Li^{+})$ (–)	Chemical shift $\delta(^{7}Li)$ (–)
0	0.00	0.00	0.00	1.00	–0.851
390	0.35	0.20	0.58	0.83	–0.648
364	0.67	0.39	1.12	0.72	–0.434
414	1.04	0.61	1.74	0.62	–0.115
367	1.37	0.80	2.28	0.56	+0.182
374	1.70	0.99	2.84	0.50	+0.524
392	2.05	1.19	3.42	0.46	+0.882
396	2.41	1.40	4.01	0.42	+1.110
400	2.76	1.61	4.60	0.38	+1.328
380	3.10	1.80	5.17	0.36	+1.472
389	3.45	2.00	5.75	0.33	+1.568
389	3.80	2.21	6.33	0.31	+1.595

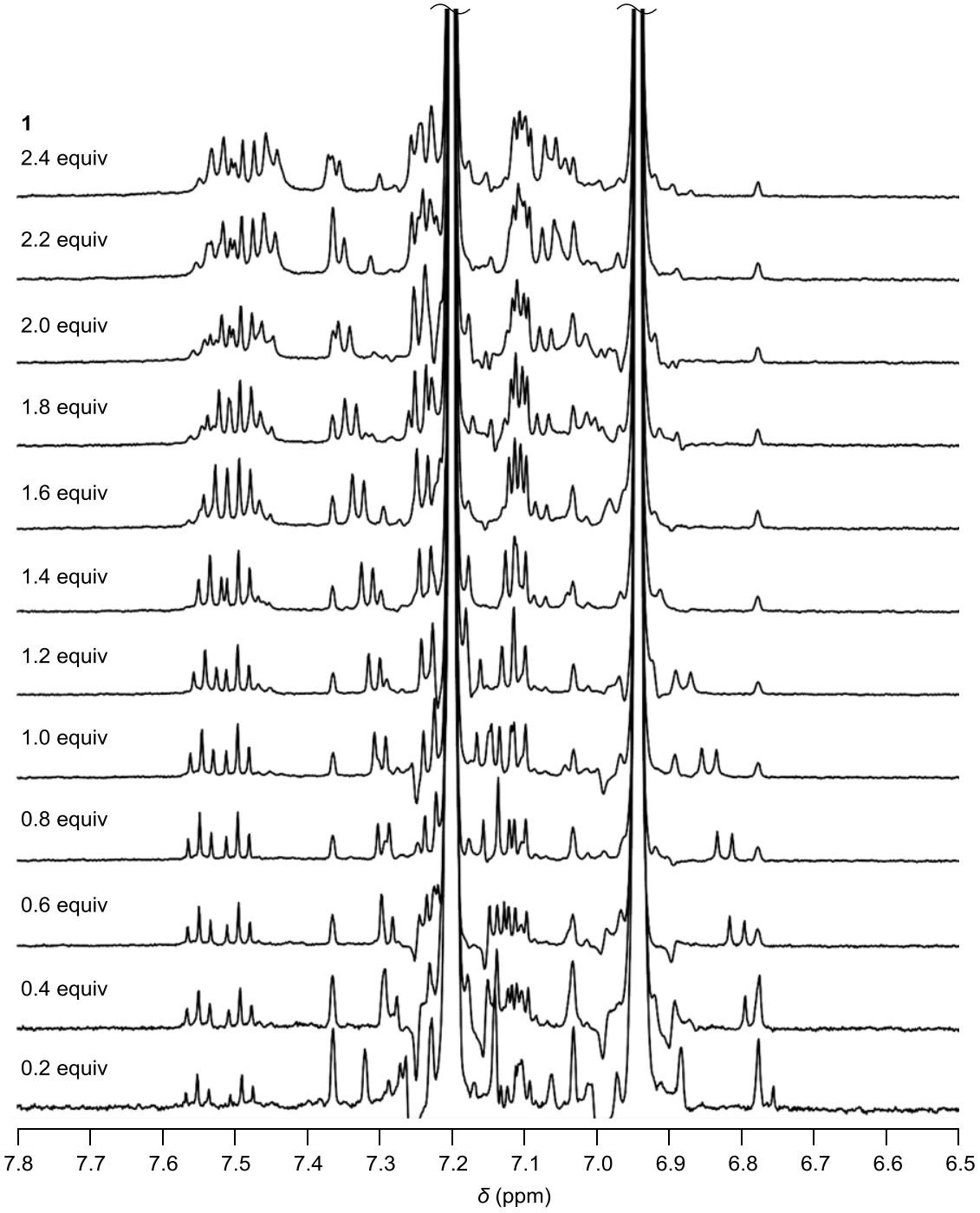


Figure S2. ^{1}H NMR spectra (500 MHz, ODCB-d_4) of **1** with $Li^{+}[B(C_6F_5)_4]^{-}$•2.5Et_2O.

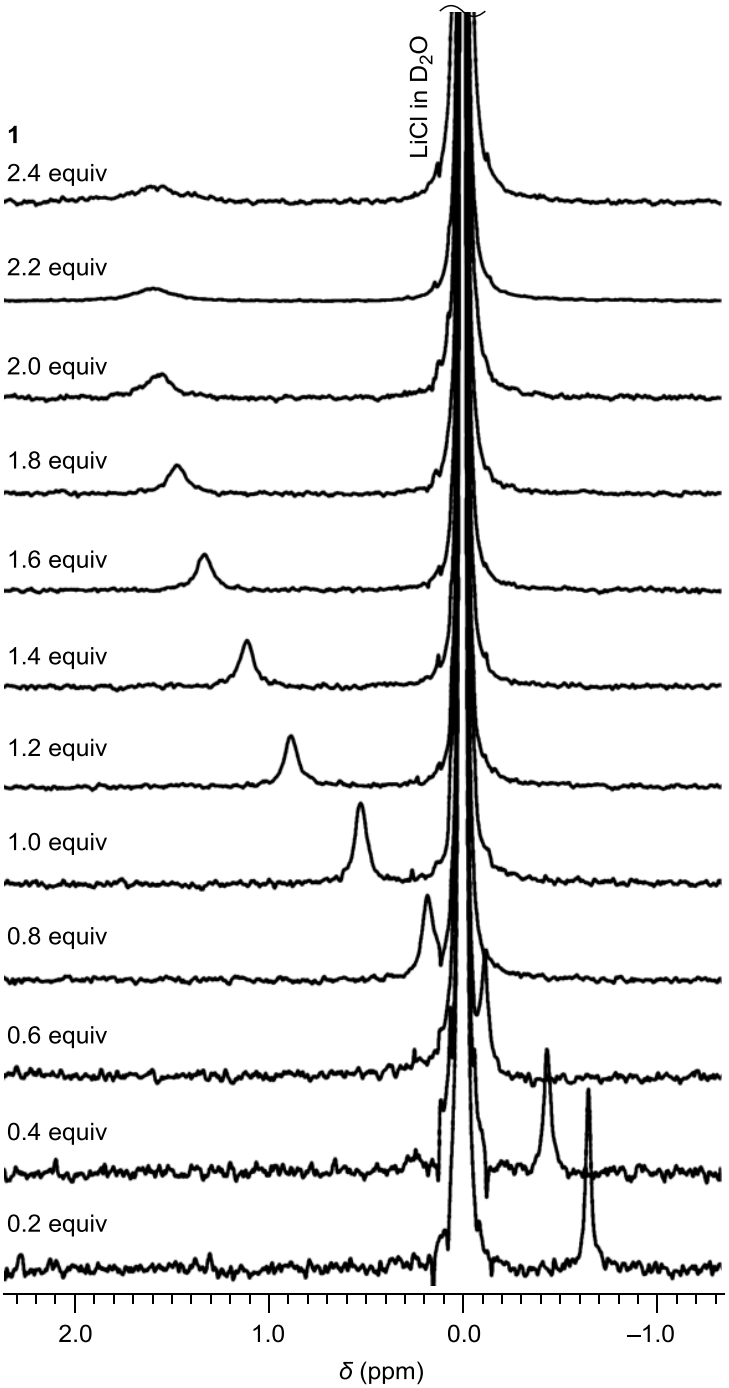


Figure S3. ^{7}Li NMR spectra (194 MHz, ODCB-d_4) of **1** with $Li^{+}[B(C_6F_5)_4]^{-}$•2.5Et_2O.

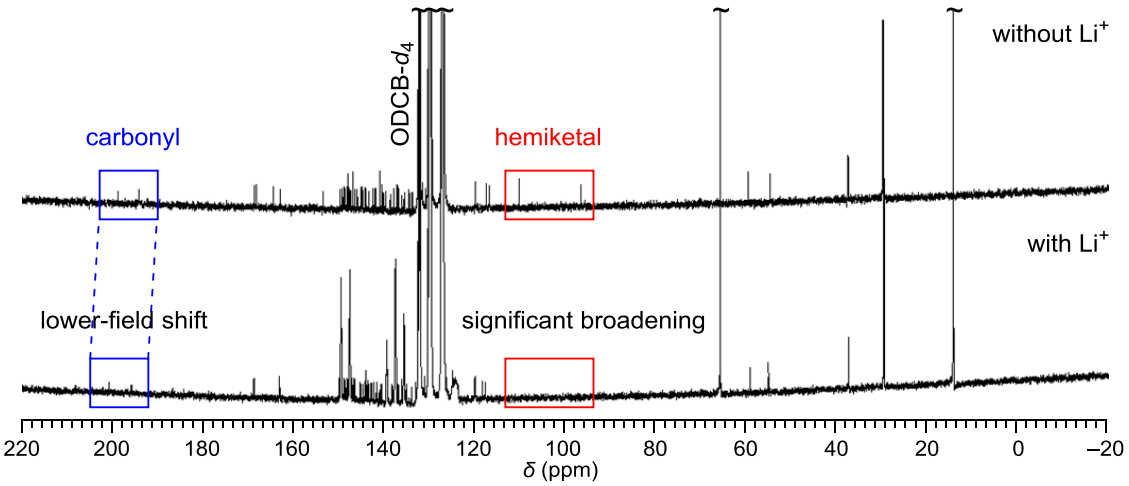


Figure S4. ^{13}C NMR spectra (126 MHz, ODCB-d_4) of **1** without and with $Li^+[B(C_6F_5)_4]^-$ •2.5Et_2O.

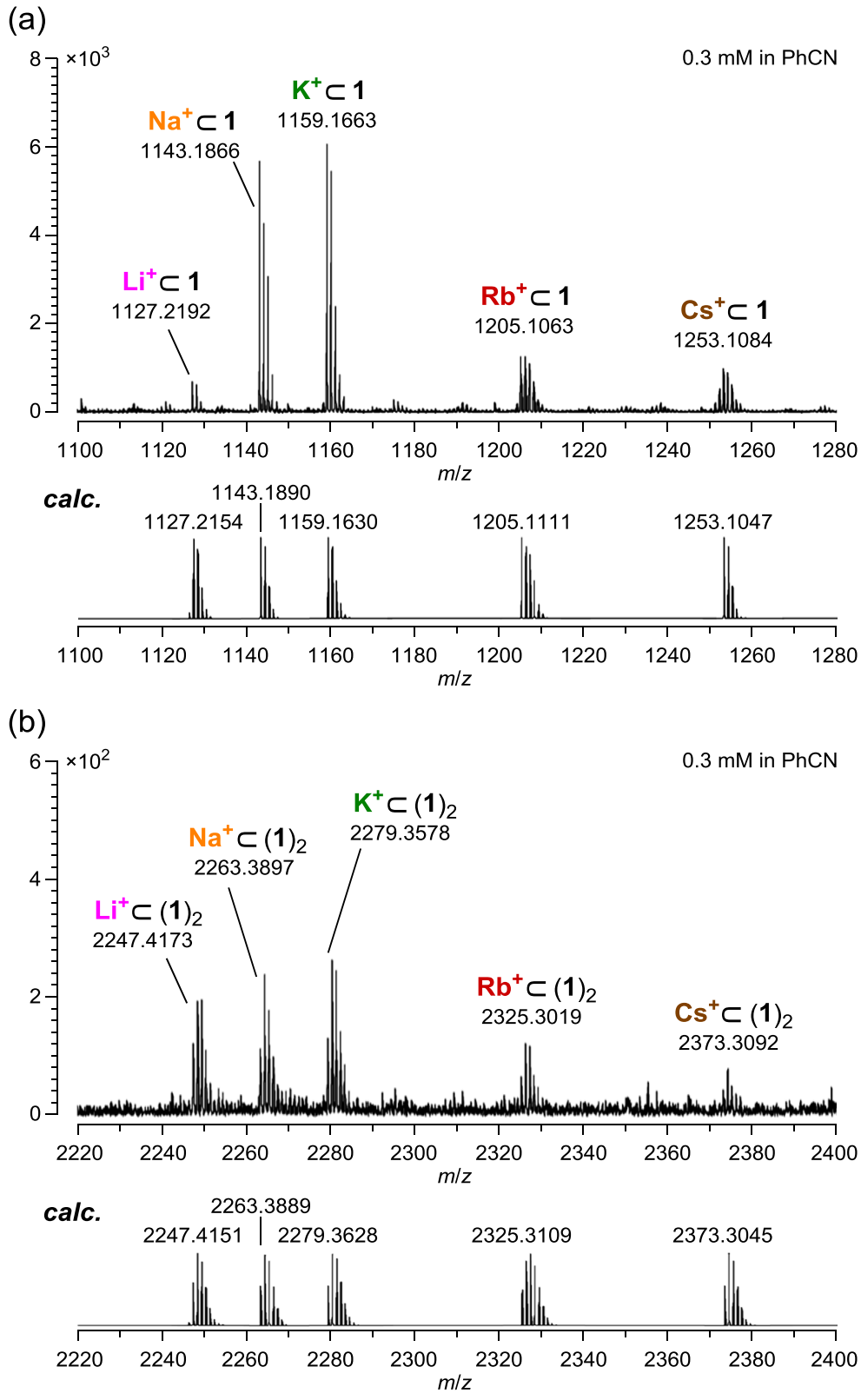


Figure S5. ESI mass spectra of **1** with $M^{+}(BPh_4)^{-}$ (M = Li, Na, K, Rb, and Cs) in benzonitrile: (a) 1:1 complexes and (b) 1:2 complexes.

4. ^{1}H NMR Relaxation Times

The sample concentration of **1** was set to 5.86 mM in ODCB-d_4 with 20 equiv of $Li^+[B(C_6F_5)_3]^-$•2.5Et_2O. Prior to measurements, the solution was degassed by three argon–vacuum cycles. The measurements were conducted on an 800 MHz NMR instrument by applying the inversion-recovery method for T_1 and CPMG method for T_2. The 90° pulse width was determined at each temperature.

Table S2. Relaxation times T_1 and T_2 with angular momentum correlation times τ_J

Temp.		**1**			$Li^+\subset$ **1**			$Li^+\subset$ (**1**)$_2$		
(°C)	(K)	T_1 (s)	T_2 (s)	τ_J (s)	T_1 (s)	T_2 (s)	τ_J (s)	T_1 (s)	T_2 (s)	τ_J (s)
17	290	3.10	0.83	0.59	4.19	0.50	0.44	4.12	0.51	0.45
27	300	2.95	1.00	0.58	3.86	0.59	0.44	3.84	0.65	0.44
37	310	2.79	1.14	0.57	3.57	0.66	0.45	3.54	0.68	0.45
47	320	2.67	1.28	0.56	3.31	0.74	0.45	3.28	0.79	0.45
57	330	2.59	1.33	0.54	3.10	0.79	0.45	3.08	0.92	0.46

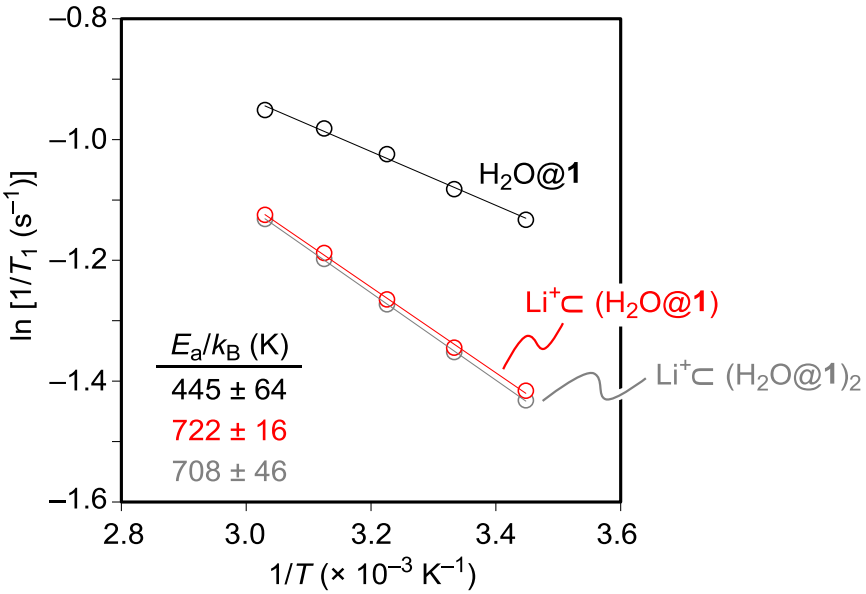
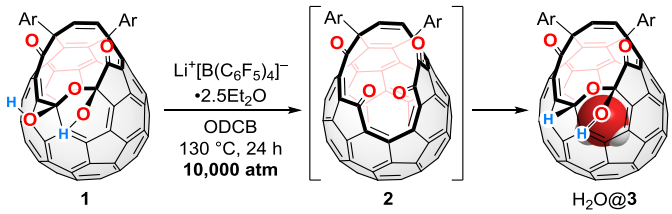


Figure S6. Arrhenius plots (ln $1/T_1$ vs. $1/T$) of H_2O@**1** with 20 equiv of $Li^+[B(C_6F_5)_3]^-$•2.5Et_2O (800 MHz, ODCB-d_4).

5. $Li^+[B(C_6F_5)_4]^-$-Mediated Selective Dehydroxyhydrogenation of 1

In the presence of $Li^+[B(C_6F_5)_3]^-$, **1** was found to be transformed into **3** under high-pressure conditions (Table S3). Without addition of the lithium salt, **3** was not formed (entries 1 and 2). The addition of the lithium salt resulted in the formation of **3** up to 34% isolated yield by increasing the amount of the lithium salt (entries 3, 4, and 6) or by extending the reaction time (entry 5). The excessive amount of water caused a lowering in a yield (entry 7). This reaction did not proceed well at ambient pressure (entry 8). When toluene was used instead of ODCB, the yield of **3** drastically decreased despite increasing the encapsulation ratio of H_2O (entry 9).



A typical procedure: Compound **1** (10.0 mg, 8.92 μmol) and $Li^+[B(C_6F_5)_3]^-$•$2.5Et_2O$ (77.8 mg, 89.3 μmol, 10.0 equiv) in ODCB (4.0 mL) were placed into a sealed vessel for the high pressure reaction. The vessel was heated at 130 °C under 10,000 atom for 24 h. After removal of ODCB under the reduced pressure, the resulting mixture was purified by silica gel column chromatography (CS_2/acetone (20:1) to (10:1)) to give H_2O@**3** (H_2O: 75%, 3.41 mg, 3.05 μmol, 34%) followed by H_2O@**1** (H_2O: 75%, 3.31 mg, 2.92 μmol, 33%).

H_2O@**3** (H_2O: 97%): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.61 (t, 1H, J = 7.74 Hz), 7.55 (t, 1H, J = 7.74 Hz), 7.41 (d, 1H, J = 7.74 Hz), 7.21 (d, 1H, J = 7.74 Hz), 7.20 (d, 1H, J = 7.74 Hz), 7.15 (d, 1H, J = 7.74 Hz), 7.02 (d, 1H, J = 10.3 Hz), 6.86 (d, 1H, J = 10.3 Hz), 1.23 (s, 9H), 1.16 (s, 9H), –9.77 (s, 1.94H); HRMS (APCI, negative ion mode) calcd for $C_{82}H_{30}N_2O_5$ (H_2O@$\mathbf{3}^{\bullet-}$) 1122.2160, found 1122.2175.

Table S3. Reaction conditions

entry	Li^+	H_2O	H_2O@**1**	H_2O@**3**	H_2O-encapsulation
1	–	excess	quant	Not formed	100%
2[a]	–	excess	81%	Not formed	25%
3	20 mol%	–	60%	6%	96%
4	1.0 equiv	–	44%	23%	94%
5[b]	1.0 equiv	–	25%	34%	85%
6	10.0 equiv	–	33%	34%	75%
7	10.0 equiv	excess	33%	17%	88%
8[a]	10.0 equiv	–	80%	trace	1.5%
9[c]	10.0 equiv	–	27%	15%	90%

[a]Conducted under 1 atm. [b]32 h. [c]Conducted in toluene.

6. Electrostatic Potential Maps

The structures of **1** and $(Li^+ \subset \mathbf{1})[B(C_6F_5)_4]^-$ were optimized at the M06-2X/6-31G(d,p) level of theory. Using these geometries, the single point calculations were conducted at the MP2/6-31G(d,p) level of theory for the visualization of the electrostatic potential maps.

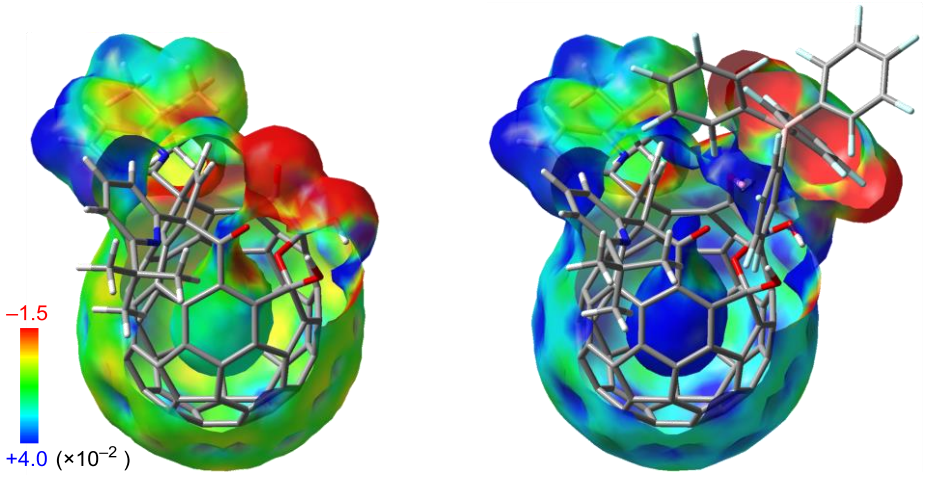
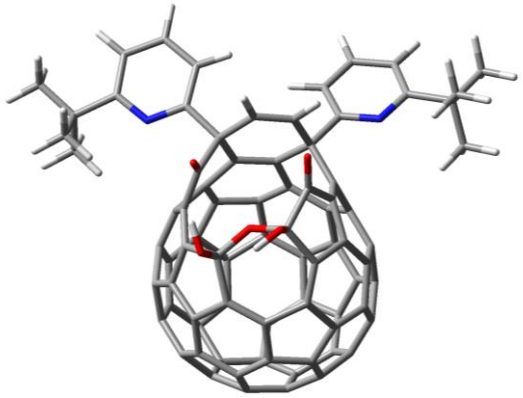


Figure S7. Electrostatic potential maps of **1** and $(Li^+ \subset \mathbf{1})[B(C_6F_5)_4]^-$ (MP2/6-31G(d,p)//M06-2X/6-31G(d,p)).

Table S4. Optimized structure of **1** (M06-2X/6-31G(d,p))

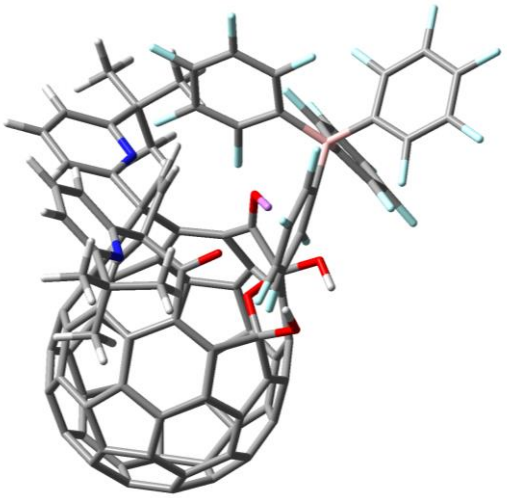


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.986361	-1.173196	-3.338560
2	6	0	-1.544961	-1.339145	-3.337206
3	6	0	-0.733473	-0.238984	-3.502632
4	6	0	-1.306405	1.082715	-3.659026
5	6	0	-2.682396	1.252403	-3.620091
6	6	0	-3.542555	0.095219	-3.454905
7	6	0	-1.187187	-2.358543	-2.369635
8	6	0	0.471267	-0.132975	-2.725070
9	6	0	-0.435007	2.003439	-2.969602
10	6	0	-3.247458	2.349502	-2.857921
11	6	0	-4.645939	0.479717	-2.595078
12	6	0	-3.535378	-2.126776	-2.402253
13	6	0	-2.405415	3.228735	-2.186254
14	6	0	-0.967781	3.055569	-2.250683
15	6	0	-2.729350	3.651858	-0.840606
16	6	0	-0.398559	3.377541	-0.959807
17	6	0	-0.034564	-2.254309	-1.575064
18	6	0	0.680234	1.264455	-2.419027
19	6	0	-1.490905	3.737510	-0.096393
20	6	0	1.306760	1.625534	-1.236933
21	6	0	0.847106	-1.108784	-1.806217
22	6	0	-4.453232	1.867198	-2.212387
23	6	0	-5.160500	-0.429277	-1.679664
24	6	0	-0.067898	-2.796098	-0.208180
25	6	0	-4.610840	-1.769202	-1.593931
26	6	0	-2.433653	-2.883308	-1.844990
27	6	0	-5.488361	0.001809	-0.333960
28	6	0	-4.637665	-2.181206	-0.207135
29	6	0	-2.486770	-3.318237	-0.539894
30	6	0	0.718316	2.711211	-0.447645
31	6	0	-4.760535	2.276022	-0.917861
32	6	0	1.795608	-0.723772	-0.786292
33	6	0	-5.149757	-1.071405	0.579088
34	6	0	-3.617606	-2.967251	0.301379
35	6	0	-1.288824	-3.292411	0.260951
36	6	0	-1.697687	-3.012862	1.610709
37	6	0	0.930225	-2.350496	0.760731
38	6	0	2.051968	0.601398	-0.536396
39	6	0	2.072730	1.960183	1.555908
40	6	0	-3.096019	-2.719619	1.625968
41	6	0	-3.526075	-1.608215	2.347286
42	6	0	-2.599412	-0.791177	3.098143
43	6	0	-4.570470	-0.776114	1.806562
44	6	0	-3.870658	3.175613	-0.215471
45	6	0	1.092653	-1.354147	3.233560
46	6	0	-5.275726	1.317919	0.043138
47	6	0	-4.677734	1.614855	1.332079
48	6	0	0.539555	-2.141590	2.066800
49	6	0	0.840925	2.571278	0.984743
50	6	0	-0.281322	2.742502	1.766272
51	6	0	-0.843856	-2.311244	2.429672
52	6	0	-1.305996	-1.229162	3.250847
53	6	0	-4.285246	0.590112	2.182162
54	6	0	-3.032529	0.630758	2.929093
55	6	0	-0.094440	-0.430987	3.685017
56	6	0	-3.820646	2.750693	1.175759
57	6	0	-1.451356	3.323069	1.226925
58	6	0	-0.672040	1.866894	2.980186
59	6	0	-2.624358	2.779366	1.874542
60	6	0	-2.215555	1.740339	2.787421
61	6	0	2.241826	-1.834485	0.152297
62	6	0	2.922929	1.070432	0.610874
63	6	0	3.496705	-0.065473	1.408285
64	6	0	3.203677	-1.343013	1.199332
65	6	0	4.044814	1.953777	0.040412
66	6	0	2.948291	-2.960647	-0.615751
67	8	0	2.399280	2.162023	2.704346
68	8	0	2.131358	-1.432511	3.820835
69	7	0	2.698779	-4.198109	-0.208857
70	6	0	3.321908	-5.228698	-0.800560
71	6	0	4.241328	-5.022856	-1.829558
72	6	0	4.511404	-3.720346	-2.243488
73	6	0	3.857903	-2.661592	-1.632073
74	6	0	5.262737	1.402650	-0.355792
75	6	0	6.212120	2.262217	-0.891428
76	6	0	5.920270	3.617399	-1.014592
77	6	0	4.670166	4.082031	-0.600446
78	7	0	3.759237	3.245319	-0.084886
79	8	0	0.048673	0.672473	2.795319
80	8	0	0.023386	-0.132211	5.017433
81	8	0	-0.388985	2.444775	4.220719
82	6	0	2.930710	-6.603741	-0.267081
83	6	0	4.222575	5.537125	-0.705869
84	6	0	3.753981	6.006972	0.679907
85	6	0	3.042344	5.599304	-1.689023
86	6	0	5.344526	6.451503	-1.201656
87	6	0	3.683072	-7.734041	-0.971844
88	6	0	1.419107	-6.783258	-0.483089
89	6	0	3.235749	-6.646078	1.238172
90	1	0	4.154416	0.218641	2.224311
91	1	0	3.620162	-2.109492	1.846446
92	1	0	4.740424	-5.858887	-2.303480
93	1	0	5.225890	-3.538636	-3.040509
94	1	0	4.033701	-1.631372	-1.926097
95	1	0	5.450138	0.340842	-0.237025
96	1	0	7.177199	1.881303	-1.211238
97	1	0	6.655666	4.297996	-1.425153

98	1	0	-0.431226	0.704357	5.195755	109	1	0	3.368182	-8.695537	-0.556081
99	1	0	0.571363	2.608242	4.211943	110	1	0	4.765637	-7.648358	-0.830818
100	1	0	3.378178	7.033243	0.618554	111	1	0	3.472127	-7.751853	-2.046149
101	1	0	4.578491	5.985185	1.399614	112	1	0	1.092017	-7.743143	-0.070564
102	1	0	2.956778	5.359337	1.052366	113	1	0	1.172367	-6.766043	-1.549686
103	1	0	2.672249	6.626708	-1.766438	114	1	0	0.867274	-5.979553	0.010825
104	1	0	2.225772	4.958519	-1.346053	115	1	0	2.914690	-7.605016	1.657463
105	1	0	3.346472	5.267533	-2.687083	116	1	0	2.709229	-5.840753	1.755019
106	1	0	4.983366	7.483243	-1.238428	117	1	0	4.308893	-6.532630	1.422875
107	1	0	5.672514	6.180161	-2.210440	---					
108	1	0	6.212052	6.424476	-0.534126	The total electronic energy was calculated to be –3625.8110624 Hartree.					

Table S5. Optimized structure of $(Li^{+}\subset\mathbf{1})[B(C_6F_5)_4]^{-}$ (M06-2X/6-31G(d,p))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.745453	0.101087	0.358188
2	6	0	-6.848770	0.618509	1.374467
3	6	0	-6.202561	-0.256570	2.219964
4	6	0	-6.391619	-1.687224	2.087491
5	6	0	-7.215393	-2.187043	1.091091
6	6	0	-7.909446	-1.270070	0.206559
7	6	0	-6.134731	1.760715	0.835331
8	6	0	-4.833034	-0.002975	2.573538
9	6	0	-5.117598	-2.308561	2.361949
10	6	0	-6.782197	-3.329665	0.310138
11	6	0	-7.915338	-1.852217	-1.122621
12	6	0	-7.629511	0.954138	-0.802647
13	6	0	-5.550623	-3.919451	0.572952
14	6	0	-4.700122	-3.398766	1.624731
15	6	0	-4.690543	-4.312632	-0.521582
16	6	0	-3.319076	-3.467779	1.193127
17	6	0	-4.787134	2.002529	1.139643
18	6	0	-4.161025	-1.278267	2.692669
19	6	0	-3.324606	-4.030695	-0.130446
20	6	0	-2.814515	-1.380606	2.381899
21	6	0	-4.138755	1.100924	2.089598
22	6	0	-7.204596	-3.116496	-1.060623
23	6	0	-7.785361	-1.035267	-2.237975
24	6	0	-3.926336	2.608023	0.109507
25	6	0	-7.660542	0.401723	-2.079419
26	6	0	-6.673058	1.994988	-0.491185
27	6	0	-6.926599	-1.435893	-3.335878
28	6	0	-6.758915	0.893398	-3.098968
29	6	0	-5.851383	2.495180	-1.476400
30	6	0	-2.369219	-2.504952	1.552908
31	6	0	-6.375372	-3.496015	-2.111323
32	6	0	-2.698397	1.043945	2.134869
33	6	0	-6.278998	-0.249053	-3.857946
34	6	0	-5.897288	1.939849	-2.816502
35	6	0	-4.482382	2.815928	-1.156880
36	6	0	-3.704357	2.550109	-2.337091
37	6	0	-2.476329	2.500599	0.232173
38	6	0	-2.055496	-0.153003	2.325125
39	6	0	-0.241015	-1.228430	1.025955
40	6	0	-4.540277	1.922659	-3.312699
41	6	0	-4.055020	0.796062	-3.970143
42	6	0	-2.725098	0.289999	-3.711571
43	6	0	-4.945873	-0.303317	-4.242841
44	6	0	-5.087898	-4.093574	-1.831446
45	6	0	-0.401951	1.678630	-1.149221
46	6	0	-6.224482	-2.628273	-3.266288
47	6	0	-4.833878	-2.675910	-3.679386
48	6	0	-1.730889	2.299655	-0.919680
49	6	0	-1.275098	-2.231219	0.638910
50	6	0	-1.393114	-2.649915	-0.676364
51	6	0	-2.396853	2.147970	-2.194732
52	6	0	-1.861830	1.055884	-2.963077
53	6	0	-4.188021	-1.527083	-4.116408
54	6	0	-2.821290	-1.205746	-3.724421
55	6	0	-0.611214	0.595590	-2.253421
56	6	0	-4.141207	-3.574929	-2.805208
57	6	0	-2.424127	-3.539012	-1.063764
58	6	0	-0.978939	-1.830375	-1.925322
59	6	0	-2.847708	-3.263144	-2.422067
60	6	0	-2.158608	-2.091759	-2.893803
61	6	0	-1.976580	2.301331	1.674124
62	6	0	-0.555353	-0.304248	2.228653
63	6	0	0.139909	1.020568	2.078307
64	6	0	-0.485261	2.161861	1.812721
65	6	0	-0.004365	-1.034952	3.463413
66	6	0	-2.382462	3.520117	2.517944
67	8	0	0.808568	-1.130744	0.412061
68	8	0	0.687164	1.840518	-0.645754
69	7	0	-2.469692	4.671765	1.865583
70	6	0	-2.774653	5.792428	2.537373
71	6	0	-2.987251	5.769639	3.916953
72	6	0	-2.875369	4.561149	4.599334
73	6	0	-2.566519	3.406282	3.895768
74	6	0	0.181934	-0.363980	4.669586
75	6	0	0.722139	-1.088502	5.722178
76	6	0	1.048570	-2.430010	5.538958
77	6	0	0.817501	-3.024316	4.296960
78	7	0	0.291133	-2.316721	3.286817
79	8	0	-0.943910	-0.506568	-1.437780

80	8	0	0.571228	0.450702	-2.942972	123	6	0	3.997876	0.752845	-2.766107
81	8	0	0.203391	-2.207763	-2.544435	124	6	0	3.175364	1.515456	-3.576575
82	6	0	-2.872824	7.049599	1.678326	125	6	0	8.594426	-0.299652	-2.947960
83	6	0	1.120541	-4.482674	3.969593	126	6	0	7.427862	-0.583598	-2.243839
84	6	0	2.022716	-4.534169	2.725986	127	6	0	6.799455	0.336727	-1.415554
85	6	0	-0.211311	-5.183727	3.654731	128	6	0	7.403570	1.590225	-1.362693
86	6	0	1.812805	-5.199093	5.130609	129	6	0	8.564333	1.917912	-2.043510
87	6	0	-3.233899	8.286100	2.503669	130	6	0	9.165860	0.957944	-2.846966
88	6	0	-3.952796	6.814862	0.609412	131	6	0	4.901367	-1.457378	-0.559950
89	6	0	-1.516978	7.271670	0.989536	132	6	0	5.753266	-2.376956	0.056721
90	3	0	1.916666	0.295209	-0.531607	133	6	0	5.402095	-3.683675	0.362117
91	1	0	1.218726	1.006686	2.186960	134	6	0	4.122600	-4.137097	0.060547
92	1	0	0.087568	3.075230	1.675943	135	6	0	3.236856	-3.265104	-0.542712
93	1	0	-3.235104	6.676444	4.454088	136	6	0	3.655774	-1.978970	-0.850286
94	1	0	-3.032790	4.523986	5.672766	137	6	0	4.174763	0.707141	3.068435
95	1	0	-2.476355	2.442947	4.387735	138	6	0	5.341889	0.915671	3.789021
96	1	0	-0.062559	0.689480	4.759131	139	6	0	6.554036	0.906442	3.117388
97	1	0	0.899767	-0.611174	6.680701	140	6	0	6.589494	0.691572	1.740732
98	1	0	1.484448	-2.998309	6.351198	141	6	0	5.447146	0.497911	0.970342
99	1	0	0.600729	-0.423491	-3.365800	142	6	0	4.272352	0.505999	1.705098
100	1	0	0.885074	-2.336176	-1.862507	143	5	0	5.385128	0.122542	-0.633420
101	1	0	2.235031	-5.573336	2.459998	144	9	0	3.076961	0.294599	1.064648
102	1	0	2.976916	-4.028706	2.912213	145	9	0	2.986271	0.698689	3.685085
103	1	0	1.535379	-4.048909	1.875425	146	9	0	5.294372	1.112904	5.104590
104	1	0	-0.028166	-6.226063	3.375413	147	9	0	7.681925	1.092661	3.799197
105	1	0	-0.718893	-4.682777	2.825548	148	9	0	7.805967	0.670556	1.192629
106	1	0	-0.875801	-5.172589	4.524818	149	9	0	6.984092	-1.989657	0.406453
107	1	0	2.022645	-6.234333	4.847636	150	9	0	6.265736	-4.503335	0.955571
108	1	0	1.183517	-5.221531	6.026268	151	9	0	3.752776	-5.378994	0.363147
109	1	0	2.765425	-4.723362	5.385385	152	9	0	1.981679	-3.654349	-0.824499
110	1	0	-3.293533	9.158076	1.846352	153	9	0	2.693051	-1.219591	-1.474700
111	1	0	-2.477817	8.496382	3.267136	154	9	0	6.849935	2.550253	-0.602249
112	1	0	-4.205328	8.173805	2.996332	155	9	0	9.103369	3.133954	-1.944031
113	1	0	-4.017644	7.683826	-0.052954	156	9	0	10.282445	1.245746	-3.513421
114	1	0	-4.933523	6.660669	1.071095	157	9	0	9.160699	-1.225185	-3.724071
115	1	0	-3.709990	5.932998	0.011332	158	9	0	6.930485	-1.818665	-2.410429
116	1	0	-1.571180	8.143173	0.329613	159	9	0	4.444616	-0.405265	-3.273496
117	1	0	-1.243617	6.397034	0.395098	160	9	0	2.800464	1.077127	-4.777790
118	1	0	-0.727980	7.449375	1.727108	161	9	0	1.805646	3.419911	-3.815366
119	6	0	2.669209	2.713711	-3.089925	162	9	0	2.505164	4.256042	-1.325052
120	6	0	3.019934	3.130985	-1.819871	163	9	0	4.093785	2.795680	0.198661
121	6	0	3.840762	2.325405	-1.031648	---					
122	6	0	4.337435	1.094363	-1.453996	The total electronic energy was calculated to be –6568.5539862 Hartree.					

7. Conformations of $Li^+ \subset 1$

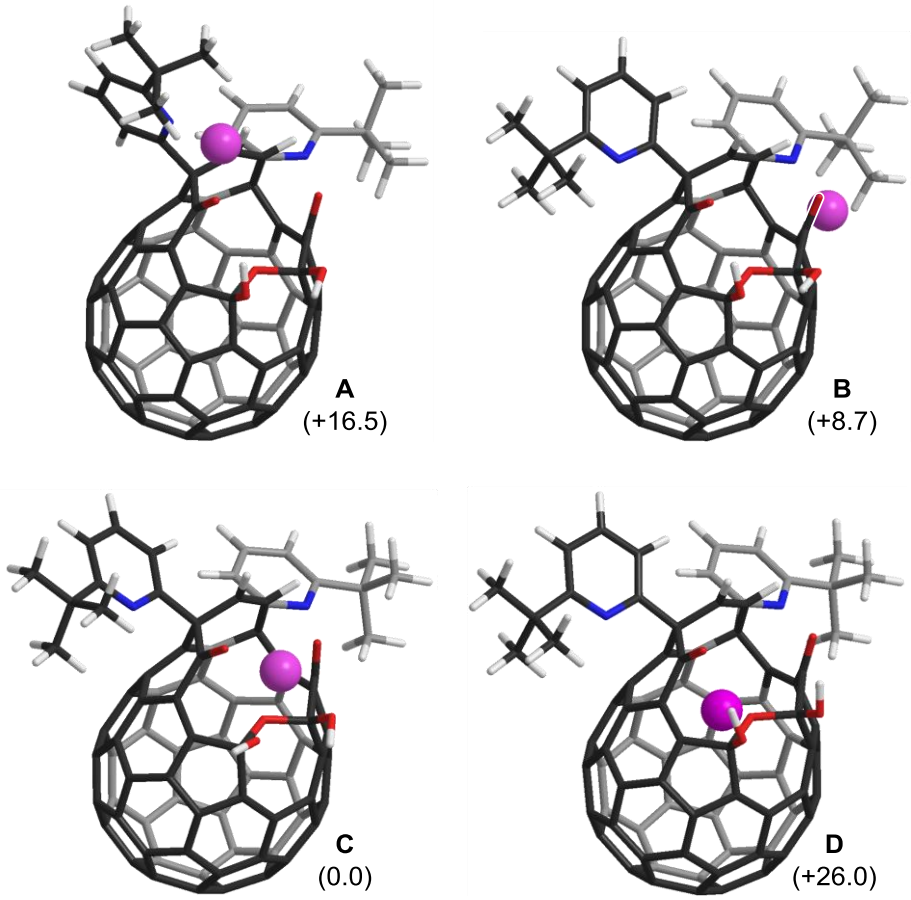
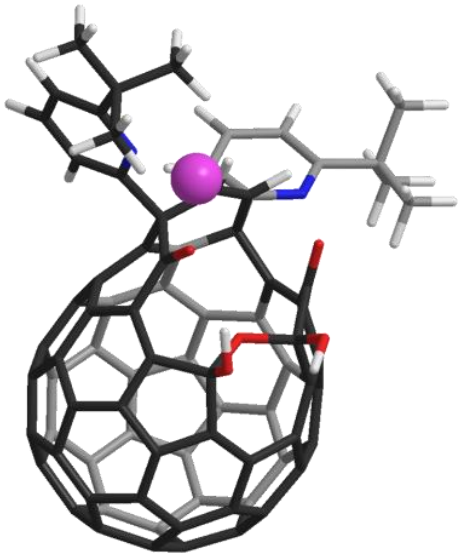


Figure S8. Optimized structures of $Li^+ \subset$ **1** with values of ΔG at 298 K (M06-2X/6-31G(d,p)).

Table S6. Optimized structure of $Li^{+}\subset$**1A** (M06-2X/6-31G(d,p))

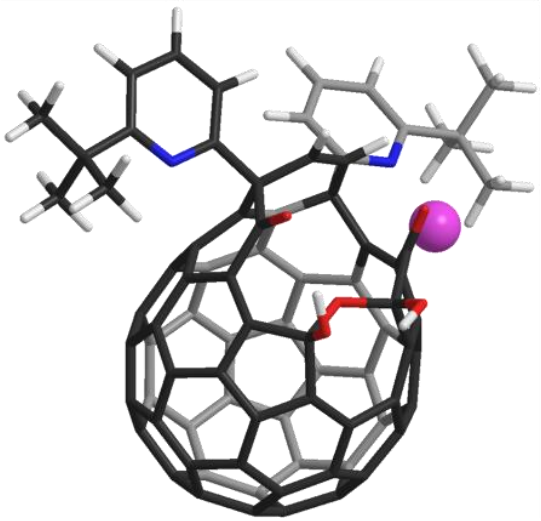


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.881302	1.273703	-2.772520
2	6	0	2.478302	1.560868	-3.006553
3	6	0	1.650684	0.570204	-3.486286
4	6	0	2.163327	-0.763325	-3.729400
5	6	0	3.492302	-1.054967	-3.462784
6	6	0	4.372617	-0.009777	-2.975149
7	6	0	2.002352	2.463598	-1.975298
8	6	0	0.316185	0.463906	-2.961720
9	6	0	1.126058	-1.690816	-3.347734
10	6	0	3.834815	-2.289112	-2.782094
11	6	0	5.268007	-0.599632	-1.998376
12	6	0	4.295796	2.040936	-1.620531
13	6	0	2.831226	-3.176195	-2.411579
14	6	0	1.445793	-2.870456	-2.705236
15	6	0	2.869324	-3.803419	-1.108443
16	6	0	0.624809	-3.306343	-1.595472
17	6	0	0.716062	2.352216	-1.427535
18	6	0	-0.027486	-0.939320	-2.907173
19	6	0	1.511360	-3.873201	-0.615519
20	6	0	-0.889609	-1.397796	-1.923470
21	6	0	-0.168166	1.331484	-1.987485
22	6	0	4.923822	-2.003768	-1.866789
23	6	0	5.650400	0.128903	-0.879959
24	6	0	0.519951	2.692296	-0.009438
25	6	0	5.174638	1.486869	-0.694788
26	6	0	3.154177	2.804017	-1.162370
27	6	0	5.694723	-0.507468	0.422777
28	6	0	4.961305	1.701536	0.719880
29	6	0	2.982720	3.048768	0.181511
30	6	0	-0.523526	-2.613759	-1.198047
31	6	0	4.958609	-2.609983	-0.614985
32	6	0	-1.322998	0.901100	-1.232189
33	6	0	5.252104	0.456838	1.410398
34	6	0	3.910963	2.493608	1.150053
35	6	0	1.654936	3.011482	0.741515
36	6	0	1.781850	2.518154	2.085450
37	6	0	-0.665469	2.201936	0.684550
38	6	0	-1.706081	-0.418004	-1.241838
39	6	0	-2.145384	-2.008031	0.612383
40	6	0	3.133839	2.111266	2.306568
41	6	0	3.357655	0.882210	2.920351
42	6	0	2.259856	0.050873	3.363733
43	6	0	4.438098	0.048206	2.458657
44	6	0	3.898037	-3.513441	-0.225619
45	6	0	-1.357632	0.869247	2.877530
46	6	0	5.340217	-1.839889	0.555118
47	6	0	4.495775	-2.257440	1.659297
48	6	0	-0.546002	1.782516	1.994886
49	6	0	-0.895716	-2.655755	0.201055
50	6	0	0.039791	-3.060958	1.141840
51	6	0	0.748930	1.787418	2.625997
52	6	0	0.987441	0.571555	3.352031
53	6	0	4.011923	-1.327945	2.570045
54	6	0	2.642442	-1.365682	3.068323
55	6	0	-0.327827	-0.170398	3.436994
56	6	0	3.617525	-3.283373	1.184173
57	6	0	1.247686	-3.659074	0.732757
58	6	0	0.258608	-2.400491	2.530411
59	6	0	2.314709	-3.310940	1.650212
60	6	0	1.808961	-2.373849	2.617927
61	6	0	-1.862520	1.911098	-0.235349
62	6	0	-2.790814	-0.967442	-0.341494
63	6	0	-3.472254	0.127042	0.448807
64	6	0	-3.055769	1.384225	0.503699
65	6	0	-3.903846	-1.721569	-1.107501
66	6	0	-2.313578	3.224966	-0.895655
67	8	0	-2.721417	-2.349365	1.647888
68	8	0	-2.516373	0.872770	3.184234
69	7	0	-2.316722	4.269945	-0.066628
70	6	0	-2.738922	5.456149	-0.505960
71	6	0	-3.195145	5.616805	-1.823943
72	6	0	-3.205542	4.524860	-2.675762
73	6	0	-2.755879	3.289740	-2.209138
74	6	0	-3.998941	-1.735989	-2.494200
75	6	0	-5.080872	-2.394768	-3.066479
76	6	0	-6.023269	-3.016278	-2.256008
77	6	0	-5.868286	-2.959385	-0.871760
78	7	0	-4.822403	-2.312476	-0.329260
79	8	0	-0.359271	-1.145668	2.394391
80	8	0	-0.751183	-0.621998	4.657775
81	8	0	-0.238759	-3.116298	3.614807
82	6	0	-2.714092	6.628689	0.470599
83	6	0	-6.834131	-3.610325	0.119166
84	6	0	-7.415201	-2.536902	1.056357
85	6	0	-6.078903	-4.676857	0.932432
86	6	0	-8.004592	-4.295290	-0.595560
87	6	0	-4.152124	7.130690	0.684147
88	6	0	-1.858176	7.761681	-0.119355
89	6	0	-2.121437	6.201397	1.815226
90	3	0	-4.552036	-2.210089	1.649956
91	1	0	-4.376506	-0.131790	0.995794
92	1	0	-3.580676	2.106429	1.121751
93	1	0	-3.537361	6.585943	-2.170347

94	1	0	-3.557979	4.628889	-3.697015	108	1	0	-7.658359	-5.091032	-1.261239
95	1	0	-2.745667	2.413060	-2.847853	109	1	0	-8.593096	-3.580937	-1.178538
96	1	0	-3.252592	-1.245893	-3.106188	110	1	0	-4.152509	7.968340	1.388208
97	1	0	-5.189120	-2.423889	-4.145846	111	1	0	-4.785293	6.338851	1.095691
98	1	0	-6.865136	-3.531887	-2.698605	112	1	0	-4.603557	7.478672	-0.249952
99	1	0	-0.184693	-1.351039	4.948452	113	1	0	-1.826669	8.602537	0.580013
100	1	0	-1.200332	-3.164368	3.494878	114	1	0	-2.263210	8.132027	-1.065667
101	1	0	-8.112837	-2.994347	1.762840	115	1	0	-0.831963	7.425364	-0.295169
102	1	0	-7.948034	-1.766487	0.492714	116	1	0	-2.102329	7.060546	2.491990
103	1	0	-6.658134	-2.014157	1.658473	117	1	0	-1.101761	5.825649	1.694764
104	1	0	-6.751188	-5.140927	1.659223	118	1	0	-2.712188	5.405563	2.275225
105	1	0	-5.220871	-4.276323	1.488991	---					
106	1	0	-5.683580	-5.459001	0.278555	The total electronic energy was calculated to be –3633.2168202 Hartree.					
107	1	0	-8.669287	-4.749199	0.143560						

Table S7. Optimized structure of $Li^{+}\subset$**1B** (M06-2X/6-31G(d,p))



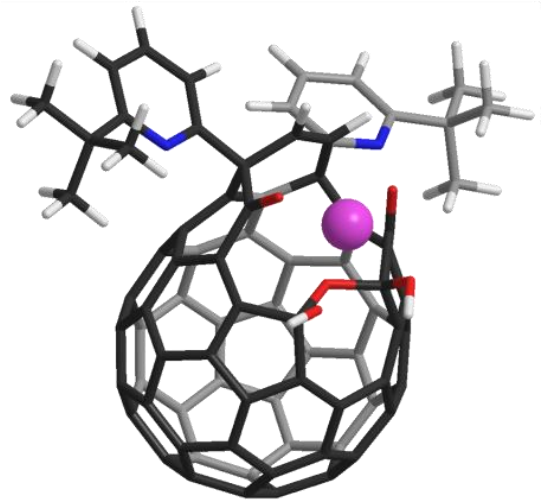
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.565596	-2.752919	-3.371665
2	6	0	-0.354146	-1.954277	-3.362624
3	6	0	-0.437980	-0.586638	-3.504922
4	6	0	-1.724805	0.062955	-3.653404
5	6	0	-2.887311	-0.692084	-3.619247
6	6	0	-2.804128	-2.133494	-3.473592
7	6	0	0.571585	-2.515065	-2.399535
8	6	0	0.420188	0.260392	-2.720942
9	6	0	-1.646543	1.318766	-2.947169
10	6	0	-4.024182	-0.224779	-2.850547
11	6	0	-3.896223	-2.558660	-2.617708
12	6	0	-1.375272	-3.848171	-2.448444
13	6	0	-3.941716	0.980172	-2.162602
14	6	0	-2.728246	1.770343	-2.217491
15	6	0	-4.461391	1.079202	-0.815574
16	6	0	-2.497437	2.364850	-0.918509
17	6	0	1.391993	-1.700835	-1.603563
18	6	0	-0.316545	1.460268	-2.395425
19	6	0	-3.566140	1.929268	-0.060406
20	6	0	-0.067153	2.121302	-1.203001
21	6	0	1.342661	-0.255130	-1.814150
22	6	0	-4.639339	-1.376560	-2.220131
23	6	0	-3.710536	-3.599842	-1.718696
24	6	0	1.690301	-2.151986	-0.236725
25	6	0	-2.427825	-4.273372	-1.642676
26	6	0	-0.048256	-3.724682	-1.885717
27	6	0	-4.238689	-3.498298	-0.371767
28	6	0	-2.183628	-4.625555	-0.260592
29	6	0	0.192002	-4.121312	-0.588310
30	6	0	-1.213650	2.563683	-0.404773
31	6	0	-5.137215	-1.277309	-0.924852
32	6	0	1.824271	0.636422	-0.784461
33	6	0	-3.288878	-4.112851	0.532279
34	6	0	-0.897257	-4.588769	0.249107
35	6	0	1.083812	-3.331872	0.223840
36	6	0	0.594077	-3.402219	1.578848
37	6	0	2.158715	-1.174903	0.751299
38	6	0	1.165589	1.810243	-0.509894
39	6	0	0.307234	2.825728	1.601260
40	6	0	-0.659786	-4.082413	1.582319
41	6	0	-1.701853	-3.507348	2.308254
42	6	0	-1.516496	-2.295084	3.076664
43	6	0	-3.036659	-3.533155	1.769357
44	6	0	-5.032515	-0.026300	-0.205669
45	6	0	1.674898	-0.365742	3.263257
46	6	0	-4.917386	-2.356374	0.021821
47	6	0	-4.650652	-1.762944	1.319025
48	6	0	1.743091	-1.302860	2.066396
49	6	0	-1.029085	2.515206	1.026646
50	6	0	-1.998919	1.915789	1.801063
51	6	0	0.796722	-2.329043	2.419380
52	6	0	-0.244487	-1.807147	3.256682
53	6	0	-3.694687	-2.308386	2.164058
54	6	0	-2.762991	-1.482833	2.923281
55	6	0	0.170039	-0.417705	3.707306
56	6	0	-4.720703	-0.339592	1.180402
57	6	0	-3.269675	1.618192	1.258195
58	6	0	-1.741899	0.981265	3.006022
59	6	0	-3.823087	0.441542	1.890199
60	6	0	-2.842588	-0.105947	2.795194
61	6	0	2.866347	0.053849	0.163959
62	6	0	1.530037	2.711274	0.651016
63	6	0	2.690114	2.196106	1.449785
64	6	0	3.286695	1.031405	1.230840
65	6	0	1.822269	4.123935	0.110893
66	6	0	4.142734	-0.354948	-0.586856
67	8	0	0.435991	3.153430	2.758927
68	8	0	2.545972	0.191134	3.859129
69	7	0	4.738749	-1.510512	-0.239803
70	6	0	5.906085	-1.862575	-0.807945
71	6	0	6.514817	-1.036719	-1.754528
72	6	0	5.902552	0.155310	-2.115429
73	6	0	4.695738	0.507714	-1.523312

74	6	0	3.120138	4.538046	-0.176885
75	6	0	3.283693	5.823327	-0.680648
76	6	0	2.168693	6.628679	-0.881529
77	6	0	0.900088	6.125495	-0.576588
78	7	0	0.752927	4.886809	-0.087217
79	8	0	-0.420663	0.518844	2.815437
80	8	0	0.072608	-0.128798	5.037971
81	8	0	-1.895995	1.582596	4.252010
82	6	0	6.567905	-3.177100	-0.393124
83	6	0	-0.396136	6.901217	-0.788668
84	6	0	-1.203358	6.884088	0.518657
85	6	0	-1.196342	6.186199	-1.890690
86	6	0	-0.137498	8.350037	-1.208413
87	6	0	7.906994	-2.861008	0.297263
88	6	0	6.814522	-4.045110	-1.639655
89	6	0	5.701164	-3.984587	0.582279
90	1	0	3.009778	2.824700	2.275652
91	1	0	4.096956	0.708143	1.878881
92	1	0	7.457715	-1.326180	-2.203592
93	1	0	6.363338	0.805534	-2.851660
94	1	0	4.184316	1.432037	-1.771363
95	1	0	3.966641	3.883152	-0.001044
96	1	0	4.275602	6.197880	-0.912769
97	1	0	2.285962	7.633313	-1.267453
98	1	0	-0.799021	0.252610	5.225921
99	1	0	-1.298955	2.352605	4.253236
100	1	0	-2.155235	7.403417	0.373171
101	1	0	-0.657973	7.387466	1.322756
102	1	0	-1.406734	5.857133	0.831524
103	1	0	-2.148946	6.699706	-2.052972
104	1	0	-1.402985	5.151358	-1.603649
105	1	0	-0.644640	6.180963	-2.836104
106	1	0	-1.091704	8.871961	-1.319238
107	1	0	0.382671	8.408886	-2.169741
108	1	0	0.451556	8.887843	-0.458683
109	1	0	8.401659	-3.788729	0.598910
110	1	0	7.756232	-2.243644	1.188049
111	1	0	8.581745	-2.325728	-0.375078
112	1	0	7.276491	-4.992461	-1.347827
113	1	0	7.488502	-3.553863	-2.344773
114	1	0	5.877979	-4.263597	-2.161741
115	1	0	6.213925	-4.910060	0.853058
116	1	0	4.753753	-4.300559	0.116294
117	1	0	5.541565	-3.447003	1.529419
118	3	0	3.716500	-2.744399	0.901808

The total electronic energy was calculated to be –3633.2055026 Hartree.

Table S8. Optimized structure of Li^{+}⊂**1C** (M06-2X/6-31G(d,p))



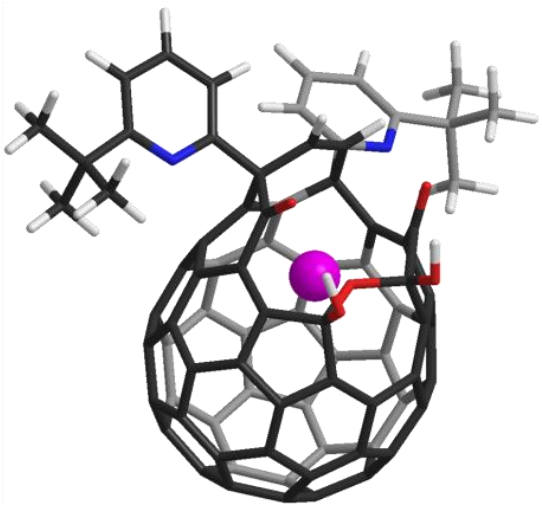
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.899633	-1.774110	-3.218961
2	6	0	2.219986	-0.493187	-3.268340
3	6	0	0.869083	-0.451697	-3.531104
4	6	0	0.118412	-1.675733	-3.733455
5	6	0	0.755359	-2.903057	-3.643833
6	6	0	2.181897	-2.952216	-3.382356
7	6	0	2.784237	0.380797	-2.257150
8	6	0	0.046834	0.482038	-2.812555
9	6	0	-1.176012	-1.480790	-3.125942
10	6	0	0.123420	-3.987580	-2.917398
11	6	0	2.434324	-4.075950	-2.500585
12	6	0	3.929361	-1.681326	-2.209662
13	6	0	-1.120498	-3.792194	-2.327330
14	6	0	-1.786812	-2.510789	-2.438697
15	6	0	-1.371119	-4.296231	-0.995456
16	6	0	-2.451062	-2.217267	-1.185636
17	6	0	1.991120	1.271534	-1.518618
18	6	0	-1.238005	-0.142027	-2.586641
19	6	0	-2.186755	-3.320045	-0.303788
20	6	0	-1.967596	0.174958	-1.453977
21	6	0	0.572493	1.346188	-1.856816
22	6	0	1.160359	-4.704513	-2.200999
23	6	0	3.412286	-3.982861	-1.519515
24	6	0	2.353317	1.550017	-0.118143
25	6	0	4.193500	-2.767822	-1.381993
26	6	0	3.884158	-0.345571	-1.653092
27	6	0	3.154980	-4.497961	-0.188683
28	6	0	4.452523	-2.552910	0.025026
29	6	0	4.183935	-0.138369	-0.325788
30	6	0	-2.567929	-0.916580	-0.682717
31	6	0	0.914038	-5.192552	-0.921893
32	6	0	-0.349168	1.914369	-0.903733
33	6	0	3.782667	-3.607632	0.767509
34	6	0	4.484906	-1.266458	0.536268
35	6	0	3.421915	0.828283	0.424744
36	6	0	3.343475	0.337889	1.774517
37	6	0	1.355339	2.125410	0.782718
38	6	0	-1.600138	1.377964	-0.745902
39	6	0	-2.814824	0.649300	1.279595
40	6	0	3.896221	-0.981222	1.824223
41	6	0	3.195147	-1.974401	2.503491
42	6	0	1.952098	-1.678513	3.174514
43	6	0	3.137771	-3.305740	1.958063
44	6	0	-0.374930	-4.967952	-0.304895
45	6	0	0.238834	1.633892	3.115921
46	6	0	1.930577	-5.073444	0.108098
47	6	0	1.262807	-4.747811	1.355999
48	6	0	1.327454	1.691195	2.101041
49	6	0	-2.618220	-0.729587	0.753909
50	6	0	-2.197221	-1.769055	1.572167
51	6	0	2.237173	0.647372	2.527640
52	6	0	1.586472	-0.362470	3.315918
53	6	0	1.828772	-3.848086	2.248947

54	6	0	1.036109	-2.842672	2.946168
55	6	0	0.230483	0.162818	3.632451
56	6	0	-0.145036	-4.685242	1.104054
57	6	0	-1.969281	-3.059076	1.041876
58	6	0	-1.329302	-1.621706	2.844532
59	6	0	-0.896844	-3.724245	1.757957
60	6	0	-0.330846	-2.805038	2.710669
61	6	0	0.241640	2.918919	0.073407
62	6	0	-2.568750	1.833316	0.319886
63	6	0	-2.053508	3.020607	1.087297
64	6	0	-0.810114	3.480428	0.993258
65	6	0	-3.925424	2.150003	-0.328962
66	6	0	0.870876	4.111294	-0.665979
67	8	0	-3.143136	0.852593	2.440936
68	8	0	-0.603845	2.390278	3.537112
69	7	0	1.975399	4.607363	-0.123095
70	6	0	2.566150	5.673799	-0.686195
71	6	0	2.024266	6.279361	-1.822210
72	6	0	0.855328	5.764527	-2.374266
73	6	0	0.257068	4.656033	-1.792365
74	6	0	-4.121249	3.333677	-1.035078
75	6	0	-5.366668	3.524028	-1.618600
76	6	0	-6.349535	2.547818	-1.475085
77	6	0	-6.065217	1.392087	-0.744987
78	7	0	-4.856642	1.213608	-0.188339
79	8	0	-0.753138	-0.349455	2.732290
80	8	0	-0.245307	0.173592	4.936753
81	8	0	-2.040742	-1.601418	4.073113
82	6	0	3.847212	6.138975	-0.001199
83	6	0	-7.059775	0.260008	-0.510209
84	6	0	-7.251237	0.095311	1.006255
85	6	0	-6.464728	-1.033530	-1.089504
86	6	0	-8.413152	0.537518	-1.167447
87	6	0	4.479820	7.337469	-0.710645
88	6	0	4.840084	4.965067	0.001354
89	6	0	3.508972	6.521979	1.448208
90	1	0	-2.754191	3.483319	1.775858
91	1	0	-0.493989	4.319079	1.607812
92	1	0	2.504714	7.137800	-2.274468
93	1	0	0.419900	6.223185	-3.256369
94	1	0	-0.648425	4.217886	-2.200010
95	1	0	-3.327722	4.069839	-1.114003
96	1	0	-5.576343	4.428121	-2.181294
97	1	0	-7.323835	2.690513	-1.925236
98	1	0	-0.246253	-0.723450	5.303347
99	1	0	-2.709657	-2.299522	4.074768
100	1	0	-7.929409	-0.739575	1.207492
101	1	0	-7.681420	0.999731	1.447538
102	1	0	-6.291909	-0.103313	1.492115
103	1	0	-7.149050	-1.869457	-0.915063
104	1	0	-5.506442	-1.259758	-0.613929
105	1	0	-6.302227	-0.943094	-2.168223
106	1	0	-9.092734	-0.295428	-0.968099
107	1	0	-8.322819	0.639124	-2.253757
108	1	0	-8.876377	1.445745	-0.769043
109	1	0	5.396778	7.625065	-0.189277
110	1	0	3.813756	8.206181	-0.711709
111	1	0	4.747099	7.100674	-1.745552
112	1	0	5.759618	5.255227	0.518708
113	1	0	5.100500	4.670799	-1.020471
114	1	0	4.407136	4.100257	0.510858
115	1	0	4.419626	6.816619	1.978544
116	1	0	3.056432	5.675448	1.970186
117	1	0	2.809316	7.363209	1.477495
118	3	0	-2.115883	0.740029	4.028130

The total electronic energy was calculated to be –3633.2331605 Hartree.

Table S9. Optimized structure of Li^{+}⊂**1D** (M06-2X/6-31G(d,p))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.122820	-0.072780	-3.381013
2	6	0	1.853896	0.630237	-3.356475
3	6	0	0.679588	-0.075706	-3.498214
4	6	0	0.699034	-1.517163	-3.648366
5	6	0	1.906720	-2.198138	-3.624123
6	6	0	3.146945	-1.457552	-3.487315
7	6	0	1.933185	1.713090	-2.395258
8	6	0	-0.456830	0.289482	-2.696333
9	6	0	-0.444429	-2.033769	-2.935480
10	6	0	2.025273	-3.423426	-2.857390
11	6	0	4.037040	-2.229886	-2.641106
12	6	0	4.013770	0.603309	-2.466130
13	6	0	0.925190	-3.913568	-2.164204
14	6	0	-0.338252	-3.205006	-2.210282
15	6	0	1.089531	-4.420609	-0.818375
16	6	0	-0.963258	-3.278977	-0.906999
17	6	0	0.845041	2.061488	-1.581128
18	6	0	-1.181517	-0.921988	-2.373911
19	6	0	-0.070173	-4.019417	-0.053510
20	6	0	-1.882953	-1.014792	-1.183038
21	6	0	-0.410471	1.338038	-1.781606
22	6	0	3.336167	-3.435028	-2.237016
23	6	0	4.878668	-1.582481	-1.746742
24	6	0	1.113658	2.555230	-0.222246
25	6	0	4.885824	-0.133619	-1.670312
26	6	0	3.296833	1.725635	-1.898595
27	6	0	5.044508	-2.099023	-0.401632
28	6	0	5.095882	0.244660	-0.289224
29	6	0	3.541581	2.116195	-0.601221
30	6	0	-1.736507	-2.238121	-0.390522
31	6	0	3.490130	-3.923439	-0.943123
32	6	0	-1.413411	1.348350	-0.733947
33	6	0	5.159193	-0.973195	0.502438

34	6	0	4.469712	1.365881	0.225835	78	7	0	-4.699164	-1.556132	-0.084658
35	6	0	2.440539	2.550676	0.220619	79	8	0	-0.218033	-0.563567	2.813746
36	6	0	2.744154	2.152103	1.569950	80	8	0	0.201353	0.145990	5.041158
37	6	0	0.038908	2.537371	0.770238	81	8	0	-0.541266	-2.390642	4.243727
38	6	0	-2.163808	0.220050	-0.469336	82	6	0	-0.034953	7.158612	-0.422557
39	6	0	-2.681644	-1.019741	1.628344	83	6	0	-5.941314	-3.499067	-0.834659
40	6	0	3.921819	1.342509	1.563063	84	6	0	-5.528795	-4.240998	0.445886
41	6	0	3.907010	0.154374	2.290534	85	6	0	-4.951392	-3.838512	-1.962332
42	6	0	2.757099	-0.238492	3.074955	86	6	0	-7.348088	-3.939733	-1.246399
43	6	0	4.538876	-1.018130	1.743867	87	6	0	-0.283260	8.474900	-1.162119
44	6	0	2.337787	-4.408490	-0.215618	88	6	0	1.394574	6.671997	-0.712356
45	6	0	-0.418899	1.710274	3.279687	89	6	0	-0.200358	7.382595	1.089290
46	6	0	4.352187	-3.230429	-0.002690	90	3	0	-0.163105	-0.004645	0.978005
47	6	0	3.712051	-3.267676	1.299874	91	1	0	-3.908260	1.394232	2.318476
48	6	0	0.353585	2.214224	2.082573	92	1	0	-2.511267	3.327736	1.925449
49	6	0	-1.765085	-2.044840	1.045408	93	1	0	-2.143812	7.203069	-2.294673
50	6	0	-0.766429	-2.620861	1.810065	94	1	0	-3.627919	5.302178	-2.872503
51	6	0	1.712745	1.847812	2.426181	95	1	0	-3.281099	3.093003	-1.731673
52	6	0	1.756530	0.683641	3.269646	96	1	0	-5.316253	1.754533	0.068075
53	6	0	3.756987	-2.166588	2.143592	97	1	0	-7.507333	0.960265	-0.858438
54	6	0	2.600362	-1.722404	2.916737	98	1	0	-7.842926	-1.461283	-1.262732
55	6	0	0.352329	0.426457	3.732187	99	1	0	-0.685234	0.438903	5.314355
56	6	0	2.482886	-3.989730	1.170778	100	1	0	-1.504221	-2.258020	4.225675
57	6	0	0.080017	-3.613242	1.264820	101	1	0	-5.549453	-5.320658	0.271111
58	6	0	-0.056378	-1.988729	3.035059	102	1	0	-6.213471	-4.014414	1.268723
59	6	0	1.382264	-3.559554	1.892757	103	1	0	-4.519001	-3.954109	0.749724
60	6	0	1.418860	-2.442329	2.807215	104	1	0	-4.960253	-4.915570	-2.155065
61	6	0	-1.389390	2.556795	0.196948	105	1	0	-3.935538	-3.543845	-1.682832
62	6	0	-3.144291	0.128458	0.688316	106	1	0	-5.219691	-3.322477	-2.889516
63	6	0	-3.201574	1.396600	1.493904	107	1	0	-7.363586	-5.024282	-1.382419
64	6	0	-2.432904	2.459414	1.277194	108	1	0	-7.656308	-3.486027	-2.193479
65	6	0	-4.529532	-0.257121	0.138789	109	1	0	-8.089067	-3.688982	-0.480786
66	6	0	-1.623046	3.862743	-0.576535	110	1	0	0.435787	9.224328	-0.821045
67	8	0	-3.001753	-1.062933	2.794667	111	1	0	-1.286520	8.866313	-0.966136
68	8	0	-1.338796	2.141864	3.913717	112	1	0	-0.156747	8.362535	-2.243668
69	7	0	-0.833711	4.876975	-0.252249	113	1	0	2.117920	7.423429	-0.382175
70	6	0	-1.006014	6.064941	-0.854995	114	1	0	1.541441	6.503659	-1.784037
71	6	0	-2.010040	6.244517	-1.809657	115	1	0	1.594913	5.736476	-0.183354
72	6	0	-2.842045	5.176733	-2.134733	116	1	0	0.515171	8.134826	1.434324
73	6	0	-2.654855	3.951934	-1.509031	117	1	0	-0.023220	6.453417	1.636044
74	6	0	-5.499758	0.703572	-0.126722	118	1	0	-1.208500	7.737254	1.324857
75	6	0	-6.712142	0.254851	-0.640006						
76	6	0	-6.900348	-1.102975	-0.868957						
77	6	0	-5.862313	-1.996456	-0.583888						

The total electronic energy was calculated to be –3633.1943228 Hartree.

8. Conformation of $M^+ \subset 1$

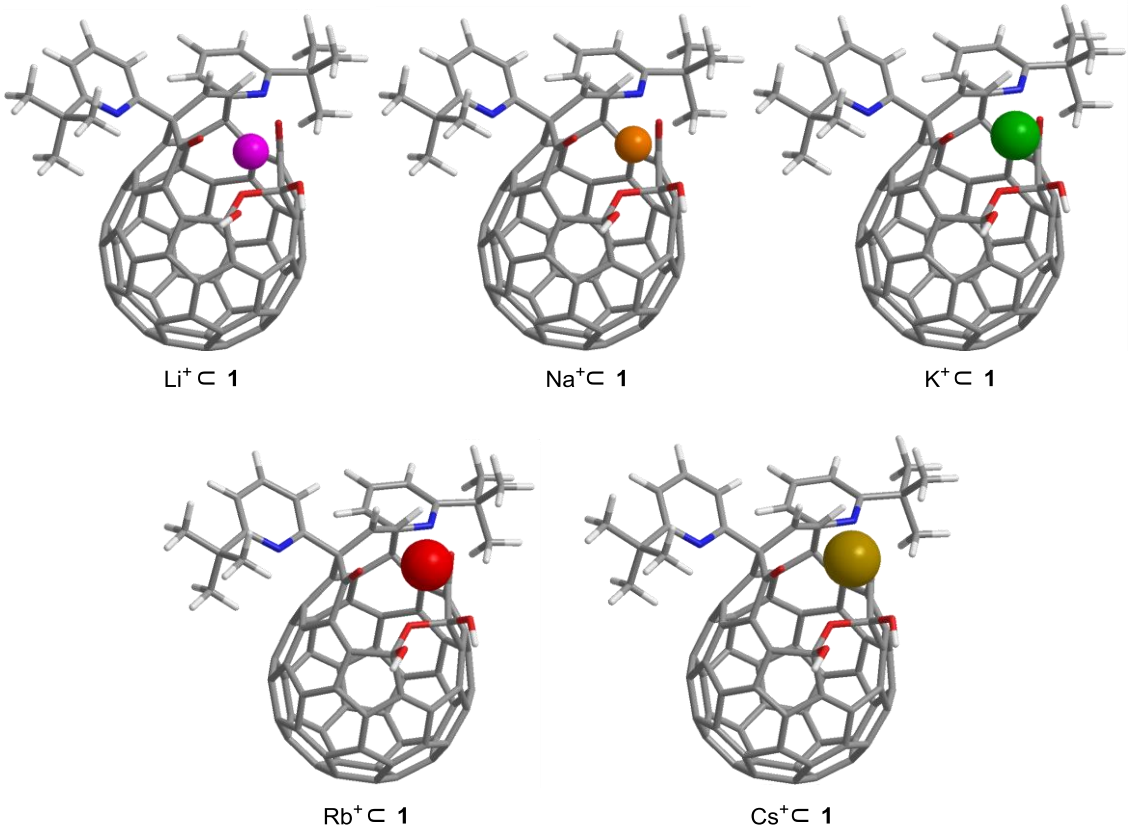
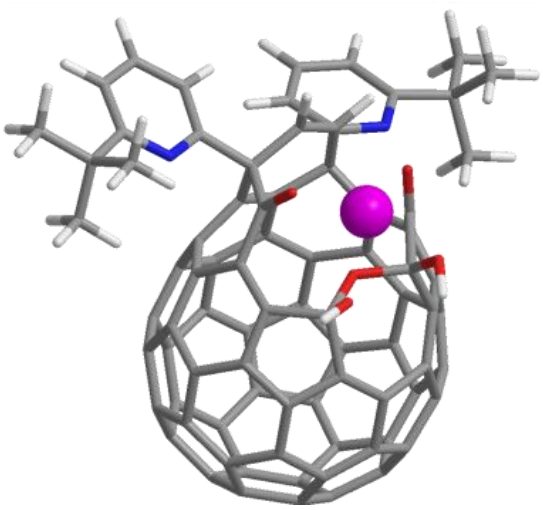


Figure S9 Optimized structures of $M^+ \subset$**1** (M06-2X/LanL2DZ for metals and 6-31G(d,p) for the rest).

Table S10. Optimized structure of $Li^{+}\subset$**1** (M06-2X/LanL2DZ for Li and 6-31G(d,p) for the rest)



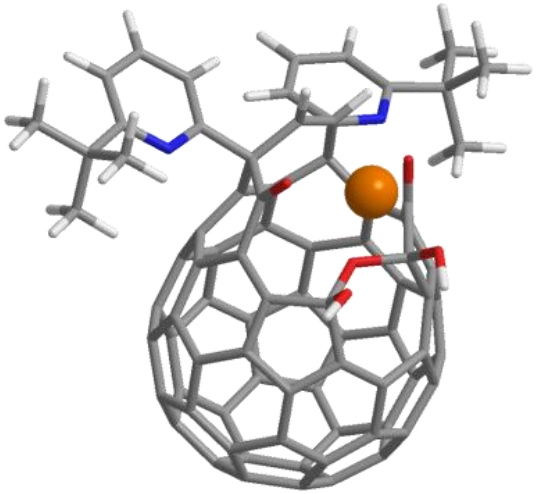
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.896228	-1.773220	-3.220614
2	6	0	2.217260	-0.492023	-3.268905
3	6	0	0.866135	-0.449719	-3.530766
4	6	0	0.114836	-1.673193	-3.733345
5	6	0	0.751261	-2.900939	-3.644802
6	6	0	2.177808	-2.950928	-3.384225
7	6	0	2.782482	0.381008	-2.257600
8	6	0	0.044776	0.484021	-2.811320
9	6	0	-1.179097	-1.477942	-3.125079
10	6	0	0.119277	-3.985516	-2.918693
11	6	0	2.430191	-4.075166	-2.503275
12	6	0	3.926575	-1.681481	-2.211976
13	6	0	-1.124242	-3.789843	-2.327787
14	6	0	-1.789985	-2.508167	-2.438093
15	6	0	-1.374326	-4.294486	-0.996136
16	6	0	-2.453220	-2.215077	-1.184560
17	6	0	1.990161	1.271644	-1.517937
18	6	0	-1.240188	-0.139469	-2.585140
19	6	0	-2.189110	-3.318423	-0.303489
20	6	0	-1.968999	0.177197	-1.451781
21	6	0	0.571469	1.347207	-1.855169
22	6	0	1.156211	-4.703272	-2.203320
23	6	0	3.408839	-3.983061	-1.522742
24	6	0	2.353291	1.548981	-0.117742
25	6	0	4.190715	-2.768594	-1.385062
26	6	0	3.882436	-0.346073	-1.654750
27	6	0	3.152070	-4.498692	-0.192152
28	6	0	4.450687	-2.554582	0.021808
29	6	0	4.183225	-0.139702	-0.327474
30	6	0	-2.569137	-0.914559	-0.680925
31	6	0	0.910410	-5.191897	-0.924285
32	6	0	-0.349298	1.915315	-0.901269
33	6	0	3.780739	-3.609260	0.764072
34	6	0	4.484070	-1.268364	0.533719
35	6	0	3.422291	0.826951	0.423965
36	6	0	3.344459	0.335900	1.773463
37	6	0	1.356015	2.124114	0.784054
38	6	0	-1.600602	1.379499	-0.743089
39	6	0	-2.814518	0.650570	1.282345
40	6	0	3.896312	-0.983542	1.822093
41	6	0	3.195052	-1.976775	2.501218
42	6	0	1.952604	-1.680740	3.173000
43	6	0	3.136652	-3.307709	1.955190
44	6	0	-0.378017	-4.967023	-0.306472
45	6	0	0.240959	1.632656	3.118277
46	6	0	1.927537	-5.073811	0.105069
47	6	0	1.260693	-4.748484	1.353418
48	6	0	1.328835	1.689397	2.102042
49	6	0	-2.618079	-0.728133	0.755564
50	6	0	-2.196908	-1.768124	1.573007
51	6	0	2.238702	0.645544	2.527408
52	6	0	1.587627	-0.364453	3.314862
53	6	0	1.827628	-3.849504	2.246559
54	6	0	1.035964	-2.844087	2.944684
55	6	0	0.232656	0.161279	3.633283
56	6	0	-0.147203	-4.685092	1.102367
57	6	0	-1.970617	-3.058248	1.042172
58	6	0	-1.328629	-1.621853	2.845016
59	6	0	-0.898206	-3.724098	1.757302
60	6	0	-0.331350	-2.805596	2.710284
61	6	0	0.242597	2.918558	0.076256
62	6	0	-2.568188	1.834806	0.323350
63	6	0	-2.051540	3.020325	1.092047
64	6	0	-0.807892	3.479640	0.997552
65	6	0	-3.924315	2.153284	-0.324890
66	6	0	0.871943	4.110821	-0.662697
67	8	0	-3.141405	0.852977	2.443901
68	8	0	-0.598701	2.390293	3.542353
69	7	0	1.978988	4.604334	-0.123125
70	6	0	2.570158	5.670165	-0.686226
71	6	0	2.026087	6.278273	-1.819887
72	6	0	0.854403	5.766279	-2.369091
73	6	0	0.255852	4.658086	-1.786696
74	6	0	-4.119599	3.339163	-1.027661
75	6	0	-5.364747	3.531723	-1.611272
76	6	0	-6.347948	2.555219	-1.471172
77	6	0	-6.063991	1.397151	-0.744489
78	7	0	-4.855975	1.217071	-0.187742
79	8	0	-0.752939	-0.349877	2.735254
80	8	0	-0.240337	0.168977	4.938671
81	8	0	-2.041617	-1.601485	4.073358
82	6	0	3.854182	6.131917	-0.004836
83	6	0	-7.058882	0.264618	-0.514483
84	6	0	-7.250657	0.093478	1.001151
85	6	0	-6.464363	-1.026591	-1.099260
86	6	0	-8.412190	0.545096	-1.170473
87	6	0	4.486627	7.330452	-0.714181
88	6	0	4.844910	4.956291	-0.007770
89	6	0	3.521655	6.512958	1.446318
90	1	0	-2.751141	3.481585	1.782661
91	1	0	-0.490685	4.316928	1.613381

92	1	0	2.506674	7.136415	-2.272545	107	1	0	-8.322031	0.650743	-2.256403
93	1	0	0.417134	6.226869	-3.249254	108	1	0	-8.875017	1.452014	-0.768660
94	1	0	-0.651777	4.222259	-2.192076	109	1	0	5.405642	7.615724	-0.195137
95	1	0	-3.325833	4.075336	-1.104084	110	1	0	3.822026	8.200257	-0.711890
96	1	0	-5.573866	4.437568	-2.171332	111	1	0	4.750418	7.094907	-1.750256
97	1	0	-7.321967	2.699533	-1.921399	112	1	0	5.766518	5.243435	0.507546
98	1	0	-0.219865	-0.725227	5.310899	113	1	0	5.101824	4.663855	-1.031007
99	1	0	-2.705430	-2.304309	4.077290	114	1	0	4.411782	4.091109	0.500917
100	1	0	-7.928736	-0.742298	1.198923	115	1	0	4.434643	6.804387	1.974396
101	1	0	-7.681027	0.996017	1.446123	116	1	0	3.068637	5.666560	1.968097
102	1	0	-6.291243	-0.106928	1.486117	117	1	0	2.824169	7.355834	1.479504
103	1	0	-7.148207	-1.863401	-0.927261	118	3	0	-2.122727	0.712031	4.047992
104	1	0	-5.505355	-1.254298	-0.625851						
105	1	0	-6.303158	-0.932006	-2.177812						
106	1	0	-9.092117	-0.288314	-0.974198						

The total electronic energy was calculated to be –3633.1910661 Hartree.

Table S11. Optimized structure of $Na^{+}\subset$**1** (M06-2X/LanL2DZ for Na and 6-31G(d,p) for the rest)



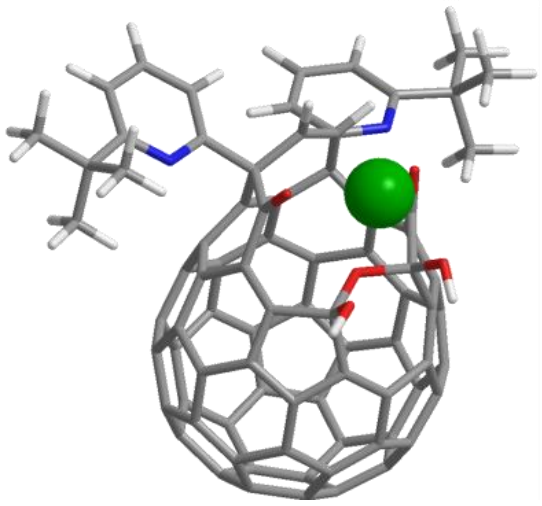
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.307241	-0.974451	-3.245956
2	6	0	2.316054	0.083935	-3.300317
3	6	0	1.001981	-0.230486	-3.564591
4	6	0	0.598300	-1.608489	-3.766061
5	6	0	1.534374	-2.626365	-3.671945
6	6	0	2.922848	-2.299726	-3.406782
7	6	0	2.629667	1.077719	-2.291587
8	6	0	-0.037959	0.457886	-2.851088
9	6	0	-0.703553	-1.757774	-3.162645
10	6	0	1.205772	-3.836826	-2.944000
11	6	0	3.457893	-3.316336	-2.521339
12	6	0	4.274823	-0.613974	-2.235200
13	6	0	-0.047479	-3.971796	-2.356577
14	6	0	-1.025762	-2.910536	-2.474180
15	6	0	-0.162600	-4.519176	-1.022538
16	6	0	-1.749151	-2.799073	-1.224881
17	6	0	1.628625	1.730733	-1.556133
18	6	0	-1.115498	-0.480759	-2.627854
19	6	0	-1.208532	-3.789143	-0.336164
20	6	0	-1.906260	-0.364326	-1.498188
21	6	0	0.240771	1.430661	-1.895476
22	6	0	2.391564	-4.255675	-2.222769
23	6	0	4.375041	-2.969388	-1.538817
24	6	0	1.902160	2.097247	-0.156078
25	6	0	4.811706	-1.592100	-1.403587
26	6	0	3.880253	0.665105	-1.683595
27	6	0	4.256307	-3.530521	-0.207084
28	6	0	5.002043	-1.313313	0.003292
29	6	0	4.111547	0.947147	-0.356641
30	6	0	-2.203395	-1.573860	-0.726663
31	6	0	2.276263	-4.787061	-0.941962
32	6	0	-0.800531	1.739576	-0.945997
33	6	0	4.629146	-2.505079	0.747635
34	6	0	4.693979	-0.061700	0.509582
35	6	0	3.121671	1.682926	0.389331
36	6	0	3.168089	1.189916	1.738662
37	6	0	0.785364	2.392608	0.741824
38	6	0	-1.866724	0.893278	-0.790222
39	6	0	-2.898721	-0.132280	1.215866
40	6	0	4.047081	0.062971	1.794784
41	6	0	3.628142	-1.076846	2.475599
42	6	0	2.347200	-1.116405	3.139584
43	6	0	3.924336	-2.378664	1.935955
44	6	0	0.972040	-4.904725	-0.328271
45	6	0	-0.160706	1.647320	3.099570
46	6	0	3.222549	-4.403708	0.089384
47	6	0	2.490135	-4.259799	1.334429
48	6	0	0.864982	1.965266	2.058947
49	6	0	-2.308953	-1.402302	0.708147
50	6	0	-1.631424	-2.284946	1.536678
51	6	0	2.014080	1.197293	2.484416
52	6	0	1.640751	0.053545	3.263643
53	6	0	2.800955	-3.242983	2.226157
54	6	0	1.770303	-2.477762	2.915279
55	6	0	0.197723	0.211876	3.605102
56	6	0	1.115084	-4.566091	1.079604
57	6	0	-1.070011	-3.470896	1.007704
58	6	0	-0.839989	-1.914691	2.820533
59	6	0	0.136615	-3.829711	1.726412
60	6	0	0.440441	-2.790608	2.675335
61	6	0	-0.495197	2.863142	0.033002
62	6	0	-2.927322	1.085441	0.265696
63	6	0	-2.726856	2.349038	1.056134
64	6	0	-1.648619	3.120172	0.964690
65	6	0	-4.307426	1.083693	-0.411331
66	6	0	-0.213017	4.179898	-0.707874
67	8	0	-3.352571	-0.046588	2.343508

68	8	0	-1.120062	2.217824	3.558385
69	7	0	0.741694	4.944073	-0.194870
70	6	0	1.020211	6.126257	-0.766436
71	6	0	0.308184	6.571457	-1.882496
72	6	0	-0.704894	5.772326	-2.404787
73	6	0	-0.979980	4.547815	-1.812862
74	6	0	-4.790029	2.225526	-1.046123
75	6	0	-6.027124	2.131163	-1.669493
76	6	0	-6.723178	0.925771	-1.634208
77	6	0	-6.162321	-0.168239	-0.971734
78	7	0	-4.963418	-0.069757	-0.376757
79	8	0	-0.650348	-0.533063	2.738044
80	8	0	-0.175370	0.090921	4.938169
81	8	0	-1.519368	-2.135633	4.047415
82	6	0	2.156294	6.907073	-0.113164
83	6	0	-6.834714	-1.531858	-0.852382
84	6	0	-7.032649	-1.836091	0.641586
85	6	0	-5.903134	-2.588678	-1.466206
86	6	0	-8.187674	-1.571732	-1.565016
87	6	0	2.428349	8.234299	-0.823369
88	6	0	3.422148	6.035506	-0.157702
89	6	0	1.776840	7.178056	1.351175
90	1	0	-3.522818	2.605462	1.749290
91	1	0	-1.555431	4.002321	1.592400
92	1	0	0.538664	7.525172	-2.340199
93	1	0	-1.269415	6.101989	-3.271295
94	1	0	-1.751963	3.888501	-2.197305
95	1	0	-4.214587	3.145550	-1.041006
96	1	0	-6.451457	2.990554	-2.178950
97	1	0	-7.690064	0.842501	-2.114350
98	1	0	0.160008	-0.744359	5.294308
99	1	0	-1.817106	-3.054724	4.083150
100	1	0	-7.470165	-2.831292	0.766230
101	1	0	-7.705749	-1.106427	1.102862
102	1	0	-6.073715	-1.802542	1.166066
103	1	0	-6.349432	-3.582638	-1.364742
104	1	0	-4.934574	-2.585928	-0.959438
105	1	0	-5.736172	-2.395099	-2.530529
106	1	0	-8.628895	-2.565972	-1.453882
107	1	0	-8.085362	-1.371976	-2.636449
108	1	0	-8.891170	-0.848519	-1.140469
109	1	0	3.249640	8.753477	-0.321967
110	1	0	1.555120	8.894079	-0.798610
111	1	0	2.720969	8.081695	-1.867259
112	1	0	4.248323	6.551226	0.341059
113	1	0	3.720085	5.831481	-1.191243
114	1	0	3.246492	5.081203	0.345700
115	1	0	2.593973	7.699783	1.858477
116	1	0	1.581013	6.238633	1.873634
117	1	0	0.880743	7.803657	1.413848
118	11	0	-2.484764	0.238557	4.385970

The total electronic energy was calculated to be –3625.8736926 Hartree.

Table S12. Optimized structure of $K^{+}\subset$**1** (M06-2X/LanL2DZ for K and 6-31G(d,p) for the rest)

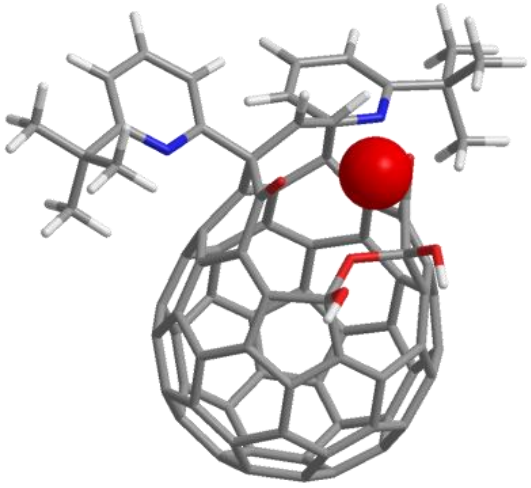


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.606963	-0.027094	-3.217330
2	6	0	2.344609	0.678606	-3.334571
3	6	0	1.196204	-0.027161	-3.615771
4	6	0	1.235031	-1.468202	-3.770857
5	6	0	2.431261	-2.151170	-3.616736
6	6	0	3.646766	-1.410964	-3.334500
7	6	0	2.310055	1.750987	-2.358435
8	6	0	-0.025938	0.335192	-2.952861
9	6	0	0.020157	-1.986606	-3.190452
10	6	0	2.460133	-3.380792	-2.848703
11	6	0	4.434186	-2.190309	-2.398469
12	6	0	4.386745	0.640245	-2.200741
13	6	0	1.288000	-3.871895	-2.284502
14	6	0	0.039185	-3.161220	-2.464729
15	6	0	1.300243	-4.385933	-0.932326
16	6	0	-0.724212	-3.236045	-1.236935
17	6	0	1.134844	2.091757	-1.671370
18	6	0	-0.775420	-0.878497	-2.715206
19	6	0	0.061154	-3.986252	-0.297484
20	6	0	-1.599595	-0.972078	-1.607461
21	6	0	-0.086290	1.377105	-2.031176
22	6	0	3.693138	-3.399093	-2.086233
23	6	0	5.171718	-1.551514	-1.411081
24	6	0	1.238677	2.564876	-0.280389
25	6	0	5.166514	-0.103053	-1.320079
26	6	0	3.606475	1.756123	-1.708352
27	6	0	5.185399	-2.081086	-0.061467
28	6	0	5.218458	0.263121	0.078435
29	6	0	3.698948	2.135545	-0.388615
30	6	0	-1.541260	-2.191071	-0.796401
31	6	0	3.702675	-3.901794	-0.788823
32	6	0	-1.203394	1.386192	-1.118306
33	6	0	5.199286	-0.962517	0.859929
34	6	0	4.531052	1.377960	0.528958
35	6	0	2.508167	2.557873	0.306163
36	6	0	2.656675	2.141307	1.673590
37	6	0	0.056591	2.530278	0.581343
38	6	0	-1.965420	0.260169	-0.949565
39	6	0	-2.720593	-0.982708	1.063407
40	6	0	3.834456	1.339141	1.793548
41	6	0	3.756959	0.146278	2.507774
42	6	0	2.527328	-0.261261	3.144012
43	6	0	4.450755	-1.019978	2.026786

44	6	0	2.475132	-4.389458	-0.199155	83	6	0	-5.959976	-3.530757	-1.133827
45	6	0	-0.692124	1.620257	2.967139	84	6	0	-6.088449	-3.883842	0.356867
46	6	0	4.455695	-3.218201	0.246628	85	6	0	-4.737352	-4.252520	-1.721941
47	6	0	3.673773	-3.265337	1.468728	86	6	0	-7.220990	-3.978836	-1.874588
48	6	0	0.216883	2.182690	1.912991	87	6	0	-0.351581	8.631675	-0.810218
49	6	0	-1.740317	-2.015649	0.627648	88	6	0	1.328259	6.906355	-0.122349
50	6	0	-0.857528	-2.622039	1.507198	89	6	0	-0.697412	7.323778	1.295316
51	6	0	1.529393	1.815277	2.389027	90	1	0	-4.131056	1.449566	1.504132
52	6	0	1.490665	0.635101	3.197622	91	1	0	-2.668453	3.373428	1.340636
53	6	0	3.633855	-2.175767	2.326836	92	1	0	-1.687971	7.338727	-2.521293
54	6	0	2.398388	-1.738471	2.963355	93	1	0	-2.788637	5.400030	-3.608102
55	6	0	0.059183	0.364693	3.528773	94	1	0	-2.586335	3.132750	-2.554181
56	6	0	2.463515	-3.980189	1.196976	95	1	0	-4.866952	1.717941	-1.317100
57	6	0	0.053144	-3.598095	1.034693	96	1	0	-6.911212	0.887964	-2.521334
58	6	0	-0.263659	-1.999067	2.803391	97	1	0	-7.450961	-1.530614	-2.455338
59	6	0	1.287435	-3.552779	1.792376	98	1	0	0.413858	-0.410161	5.264950
60	6	0	1.231595	-2.440844	2.705442	99	1	0	-0.735443	-3.377031	4.103679
61	6	0	-1.282519	2.572180	-0.170375	100	1	0	-6.205705	-4.965470	0.475666
62	6	0	-3.068751	0.151373	0.072669	101	1	0	-6.961629	-3.394586	0.800336
63	6	0	-3.277183	1.430980	0.833004	102	1	0	-5.196652	-3.562198	0.901723
64	6	0	-2.480965	2.489862	0.736485	103	1	0	-4.864440	-5.335770	-1.632187
65	6	0	-4.360668	-0.270681	-0.646965	104	1	0	-3.828447	-3.960559	-1.189425
66	6	0	-1.392434	3.904740	-0.926423	105	1	0	-4.609636	-4.009731	-2.781654
67	8	0	-3.255435	-1.034982	2.153814	106	1	0	-7.344997	-5.059436	-1.762709
68	8	0	-1.764514	1.945925	3.410008	107	1	0	-7.159334	-3.761539	-2.945703
69	7	0	-0.811133	4.940640	-0.334681	108	1	0	-8.118723	-3.498531	-1.472416
70	6	0	-0.903293	6.157676	-0.890660	109	1	0	0.186636	9.391752	-0.237266
71	6	0	-1.614938	6.354272	-2.076679	110	1	0	-1.405853	8.925287	-0.842915
72	6	0	-2.232720	5.265778	-2.685469	111	1	0	0.045990	8.643847	-1.830033
73	6	0	-2.126459	4.008118	-2.106582	112	1	0	1.886275	7.660647	0.440887
74	6	0	-5.140219	0.667620	-1.319687	113	1	0	1.736057	6.866018	-1.137496
75	6	0	-6.268249	0.200444	-1.980790	114	1	0	1.478586	5.931176	0.348639
76	6	0	-6.571152	-1.158048	-1.945789	115	1	0	-0.152031	8.083703	1.863230
77	6	0	-5.729943	-2.027336	-1.248081	116	1	0	-0.569463	6.356821	1.787305
78	7	0	-4.639658	-1.568210	-0.615667	117	1	0	-1.760603	7.584065	1.310932
79	8	0	-0.525593	-0.632079	2.699699	118	19	0	-2.822859	-0.391770	4.572972
80	8	0	-0.234701	0.191358	4.874332	---					
81	8	0	-0.860014	-2.422265	4.017190	The total electronic energy was calculated to be –3653.7689441 Hartree.					
82	6	0	-0.166549	7.266390	-0.145496						

Table S13. Optimized structure of $Rb^{+}\subset$**1** (M06-2X/LanL2DZ for Rb and 6-31G(d,p) for the rest)

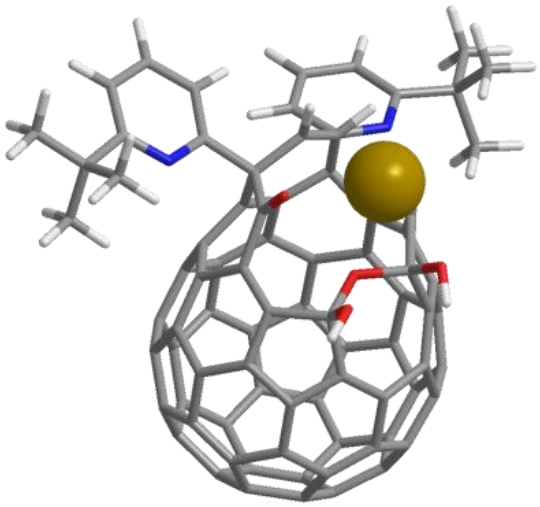


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.957888	-0.214366	-3.013949
2	6	0	2.752865	0.564992	-3.230579
3	6	0	1.593424	-0.071330	-3.614622
4	6	0	1.562531	-1.511028	-3.781683
5	6	0	2.699994	-2.262995	-3.534942
6	6	0	3.927938	-1.597244	-3.142975
7	6	0	2.696903	1.631227	-2.248982
8	6	0	0.341833	0.357052	-3.053835
9	6	0	0.275035	-1.962218	-3.313246
10	6	0	2.593242	-3.498054	-2.781605
11	6	0	4.587060	-2.427265	-2.152674
12	6	0	4.684890	0.400215	-1.927162
13	6	0	1.351158	-3.923969	-2.324244
14	6	0	0.164986	-3.141112	-2.602485
15	6	0	1.218233	-4.447101	-0.982048
16	6	0	-0.702987	-3.179555	-1.444791
17	6	0	1.488520	2.036323	-1.661270
18	6	0	-0.493793	-0.812922	-2.894462
19	6	0	-0.045668	-3.979950	-0.450241

20	6	0	-1.412802	-0.866482	-1.861025	71	6	0	-0.925382	6.422497	-2.312535
21	6	0	0.262716	1.395447	-2.129852	72	6	0	-1.590882	5.379342	-2.950080
22	6	0	3.753361	-3.592698	-1.918004	73	6	0	-1.627694	4.126714	-2.353133
23	6	0	5.271571	-1.838540	-1.098154	74	6	0	-4.889025	1.015846	-1.808161
24	6	0	1.500583	2.494449	-0.262104	75	6	0	-5.974593	0.638487	-2.587558
25	6	0	5.342283	-0.392860	-0.991921	76	6	0	-6.325744	-0.705785	-2.670114
26	6	0	3.930885	1.556270	-1.490406	77	6	0	-5.574413	-1.651491	-1.968516
27	6	0	5.139564	-2.376414	0.241637	78	7	0	-4.526345	-1.278629	-1.218610
28	6	0	5.295217	-0.038972	0.409974	79	8	0	-0.704227	-0.615391	2.526201
29	6	0	3.931339	1.921066	-0.163666	80	8	0	-0.541320	0.183205	4.725505
30	6	0	-1.493658	-2.092307	-1.063061	81	8	0	-1.232392	-2.400809	3.791353
31	6	0	3.623162	-4.102745	-0.629826	82	6	0	0.447871	7.246367	-0.288893
32	6	0	-0.925331	1.461585	-1.313140	83	6	0	-5.855106	-3.150688	-1.990464
33	6	0	5.139405	-1.266047	1.173217	84	6	0	-6.065815	-3.625773	-0.544048
34	6	0	4.636707	1.110824	0.813110	85	6	0	-4.626461	-3.858639	-2.583428
35	6	0	2.712286	2.408859	0.431342	86	6	0	-7.090921	-3.495368	-2.823866
36	6	0	2.718326	1.974612	1.801325	87	6	0	0.503069	8.586520	-1.024084
37	6	0	0.249208	2.523789	0.495829	88	6	0	1.877763	6.730284	-0.060539
38	6	0	-1.761754	0.380562	-1.221882	89	6	0	-0.248098	7.435025	1.068256
39	6	0	-2.765991	-0.836331	0.698797	90	1	0	-4.047704	1.672530	1.065356
40	6	0	3.833158	1.104352	2.012901	91	1	0	-2.473562	3.513038	1.041257
41	6	0	3.625641	-0.085812	2.704842	92	1	0	-0.879515	7.400556	-2.775065
42	6	0	2.323527	-0.425380	3.227353	93	1	0	-2.069121	5.543364	-3.910592
43	6	0	4.291339	-1.287046	2.271734	94	1	0	-2.124177	3.284237	-2.824205
44	6	0	2.324091	-4.522938	-0.151629	95	1	0	-4.579076	2.051619	-1.715467
45	6	0	-0.749928	1.651520	2.804708	96	1	0	-6.545716	1.385785	-3.129433
46	6	0	4.322281	-3.470760	0.473804	97	1	0	-7.172229	-1.008976	-3.273111
47	6	0	3.437587	-3.480327	1.624753	98	1	0	0.016314	-0.485853	5.145526
48	6	0	0.274736	2.155986	1.830172	99	1	0	-1.147403	-3.359949	3.877625
49	6	0	-1.804968	-1.915870	0.340513	100	1	0	-6.218384	-4.709237	-0.526172
50	6	0	-1.037371	-2.576328	1.286034	101	1	0	-6.946257	-3.149217	-0.100930
51	6	0	1.516547	1.708321	2.412472	102	1	0	-5.193709	-3.381256	0.068070
52	6	0	1.336922	0.526865	3.199479	103	1	0	-4.784770	-4.941475	-2.587872
53	6	0	3.386719	-2.395239	2.487942	104	1	0	-3.734503	-3.637071	-1.991558
54	6	0	2.128299	-1.891100	3.020873	105	1	0	-4.446815	-3.534761	-3.613520
55	6	0	-0.133660	0.341786	3.408565	106	1	0	-7.256987	-4.575797	-2.798103
56	6	0	2.216137	-4.121524	1.242487	107	1	0	-6.966580	-3.205692	-3.872155
57	6	0	-0.146114	-3.599649	0.880666	108	1	0	-7.991442	-3.011307	-2.432256
58	6	0	-0.523129	-1.994804	2.635379	109	1	0	1.069995	9.306250	-0.427166
59	6	0	1.019637	-3.629459	1.739710	110	1	0	-0.496453	9.003569	-1.183609
60	6	0	0.949419	-2.521014	2.655659	111	1	0	1.001731	8.494675	-1.994392
61	6	0	-1.017496	2.646320	-0.364600	112	1	0	2.444003	7.449742	0.538769
62	6	0	-2.953243	0.330129	-0.298563	113	1	0	2.399659	6.591979	-1.012928
63	6	0	-3.145457	1.611549	0.463119	114	1	0	1.857919	5.771368	0.463634
64	6	0	-2.288107	2.626173	0.441287	115	1	0	0.309225	8.153388	1.677330
65	6	0	-4.200699	0.006021	-1.138992	116	1	0	-0.299592	6.484465	1.604802
66	6	0	-0.985884	3.981382	-1.124027	117	1	0	-1.265798	7.816145	0.936545
67	8	0	-3.414269	-0.878047	1.725467	118	37	0	-3.341220	-0.180969	4.350279
68	8	0	-1.817933	2.067028	3.175974	----------					
69	7	0	-0.368036	4.977219	-0.501549	The total electronic energy was calculated to be –3649.4824661 Hartree.					
70	6	0	-0.317703	6.188027	-1.076809						

Table S14. Optimized structure of $Cs^{+}\subset$**1** (M06-2X/LanL2DZ for Cs and 6-31G(d,p) for the rest)



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.475941	0.092005	-2.609966
2	6	0	3.251064	0.767291	-2.996597
3	6	0	2.207098	0.036100	-3.517301
4	6	0	2.313531	-1.402511	-3.660765
5	6	0	3.465443	-2.057055	-3.253106
6	6	0	4.573603	-1.289973	-2.715706
7	6	0	2.981011	1.833817	-2.051270
8	6	0	0.861911	0.365263	-3.132459
9	6	0	1.014999	-1.952657	-3.355988
10	6	0	3.359567	-3.290493	-2.497571
11	6	0	5.160954	-2.054974	-1.632524
12	6	0	5.001218	0.773139	-1.449018
13	6	0	2.106085	-3.811712	-2.198067
14	6	0	0.908005	-3.130454	-2.643349
15	6	0	1.839707	-4.333235	-0.875027
16	6	0	-0.099166	-3.231566	-1.608701
17	6	0	1.677563	2.143847	-1.634068
18	6	0	0.108338	-0.866463	-3.061590
19	6	0	0.483297	-3.968536	-0.522385
20	6	0	-0.932029	-0.986162	-2.155693
21	6	0	0.578792	1.401866	-2.247371
22	6	0	4.400077	-3.283017	-1.487442
23	6	0	5.651745	-1.403143	-0.509230
24	6	0	1.469063	2.612111	-0.253600
25	6	0	5.591023	0.044058	-0.421413
26	6	0	4.106174	1.867533	-1.136865
27	6	0	5.388160	-1.938935	0.811956
28	6	0	5.331839	0.404174	0.955817
29	6	0	3.902809	2.241201	0.172142
30	6	0	-1.017717	-2.209549	-1.353581
31	6	0	4.142151	-3.790892	-0.218358
32	6	0	-0.708961	1.380025	-1.596620
33	6	0	5.175064	-0.825234	1.715256
34	6	0	4.535780	1.499225	1.247589
35	6	0	2.581343	2.632172	0.594161
36	6	0	2.440915	2.210268	1.960860
37	6	0	0.131790	2.541984	0.333752
38	6	0	-1.461261	0.233628	-1.591201
39	6	0	-2.605107	-1.049691	0.207528
40	6	0	3.584318	1.436424	2.332680
41	6	0	3.382909	0.238953	3.013892
42	6	0	2.054631	-0.202025	3.368767
43	6	0	4.193711	-0.907240	2.693140
44	6	0	2.829141	-4.312558	0.093818
45	6	0	-1.093002	1.616642	2.515076
46	6	0	4.637977	-3.094941	0.955255
47	6	0	3.612755	-3.168534	1.980200
48	6	0	0.008797	2.187870	1.666134
49	6	0	-1.522864	-2.049020	-0.006294
50	6	0	-0.836838	-2.636867	1.043123
51	6	0	1.194149	1.850111	2.414583
52	6	0	1.006117	0.665428	3.194374
53	6	0	3.361079	-2.084251	2.808669
54	6	0	2.007086	-1.680296	3.163571
55	6	0	-0.461292	0.360496	3.211206
56	6	0	2.507280	-3.910723	1.454118
57	6	0	0.178965	-3.587100	0.776825
58	6	0	-0.551941	-2.000291	2.434801
59	6	0	1.220082	-3.514629	1.781516
60	6	0	0.941517	-2.406424	2.657643
61	6	0	-1.015928	2.557893	-0.686343
62	6	0	-2.752304	0.093457	-0.823163
63	6	0	-3.137955	1.357731	-0.108246
64	6	0	-2.370458	2.439386	-0.043278
65	6	0	-3.858202	-0.329729	-1.805383
66	6	0	-0.997563	3.895720	-1.439759
67	8	0	-3.377220	-1.141418	1.139628
68	8	0	-2.221173	1.965938	2.748150
69	7	0	-0.634029	4.943673	-0.710245
70	6	0	-0.633670	6.166249	-1.260571
71	6	0	-1.025471	6.356948	-2.587920
72	6	0	-1.422086	5.256935	-3.342328
73	6	0	-1.412707	3.993294	-2.766562
74	6	0	-4.530747	0.620534	-2.570912
75	6	0	-5.487170	0.158273	-3.465245
76	6	0	-5.731355	-1.208762	-3.562601
77	6	0	-5.003788	-2.090135	-2.759755
78	7	0	-4.080971	-1.635153	-1.899011
79	8	0	-0.820132	-0.641441	2.270461
80	8	0	-1.022140	0.167930	4.463806
81	8	0	-1.369659	-2.452072	3.499116
82	6	0	-0.170628	7.288883	-0.337206
83	6	0	-5.173003	-3.605888	-2.784878
84	6	0	-5.510398	-4.080025	-1.362337
85	6	0	-3.837851	-4.228615	-3.223218
86	6	0	-6.279833	-4.047417	-3.743962
87	6	0	-0.187377	8.652350	-1.030134
88	6	0	1.260163	6.967073	0.123608
89	6	0	-1.101846	7.326176	0.884871
90	1	0	-4.106658	1.345303	0.383648
91	1	0	-2.693919	3.311407	0.518464

92	1	0	-1.021865	7.345808	-3.029307	107	1	0	-6.058121	-3.762317	-4.777315
93	1	0	-1.731857	5.386744	-4.374558	108	1	0	-7.249701	-3.622559	-3.465349
94	1	0	-1.706530	3.109969	-3.324441	109	1	0	0.155556	9.419828	-0.330751
95	1	0	-4.307553	1.676890	-2.461928	110	1	0	-1.195288	8.928238	-1.356666
96	1	0	-6.041421	0.856228	-4.084918	111	1	0	0.478663	8.673987	-1.898628
97	1	0	-6.476126	-1.579784	-4.255294	112	1	0	1.607998	7.730446	0.826351
98	1	0	-0.494821	-0.491077	4.936132	113	1	0	1.948900	6.945761	-0.727025
99	1	0	-1.200859	-3.395823	3.622928	114	1	0	1.291523	5.992148	0.616935
100	1	0	-5.591063	-5.171194	-1.342717	115	1	0	-0.766276	8.096731	1.585778
101	1	0	-6.464642	-3.660840	-1.026764	116	1	0	-1.098494	6.360329	1.395832
102	1	0	-4.730177	-3.770094	-0.662033	117	1	0	-2.129321	7.559083	0.587436
103	1	0	-3.916002	-5.320246	-3.222067	118	55	0	-3.956977	-0.411073	3.906027
104	1	0	-3.036201	-3.933506	-2.540902	---					
105	1	0	-3.567727	-3.906044	-4.233655	The total electronic energy was calculated to be –3645.4956394 Hartree.					
106	1	0	-6.373977	-5.136422	-3.715201						

9. Conformations of $[Li^+\subset(H_2O@1)][B(C_6F_5)_4]^-$

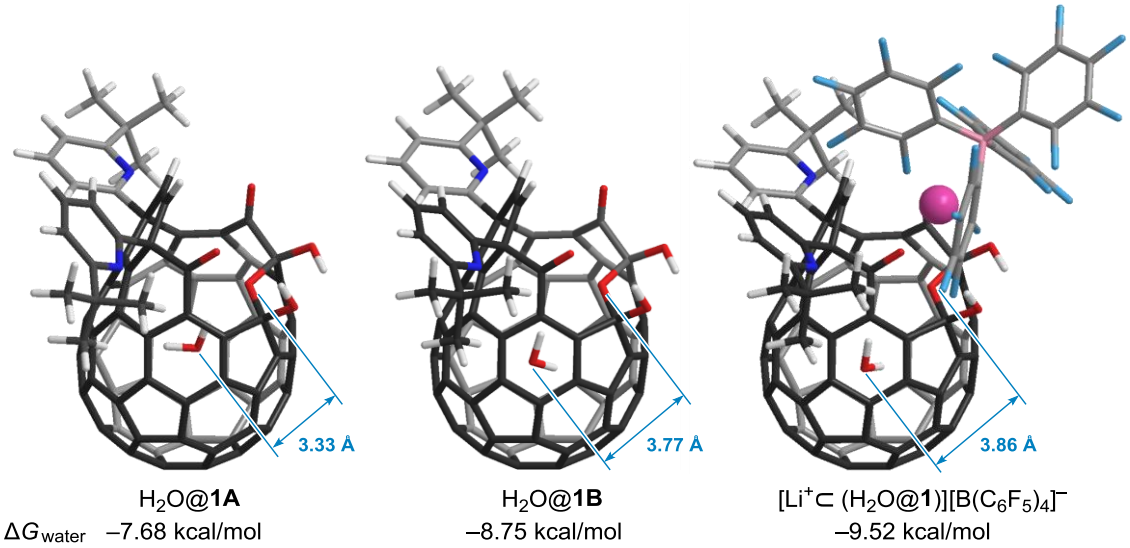


Figure S10. Optimized structures of $H_2O@\mathbf{1}$ and $[Li^+\subset(H_2O@\mathbf{1})][B(C_6F_5)_4]^-$ (M06-2X/6-31G(d,p), 298 K). The ΔG values represent the stabilization energies induced by the H_2O-insertion.

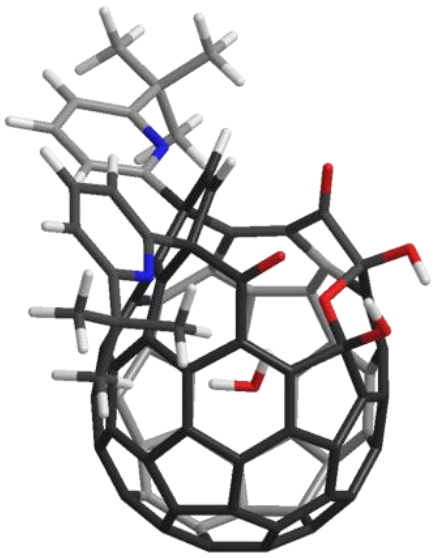
Table S15. Optimized structure of H_2O (M06-2X/6-31G(d,p))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.117808
2	1	0	0.000000	0.760256	-0.471232
3	1	0	0.000000	-0.760256	-0.471232

The total electronic energy was calculated to be –76.3839203 Hartree.

Table S16. Optimized structure of H_2O@**1A** (M06-2X/6-31G(d,p))



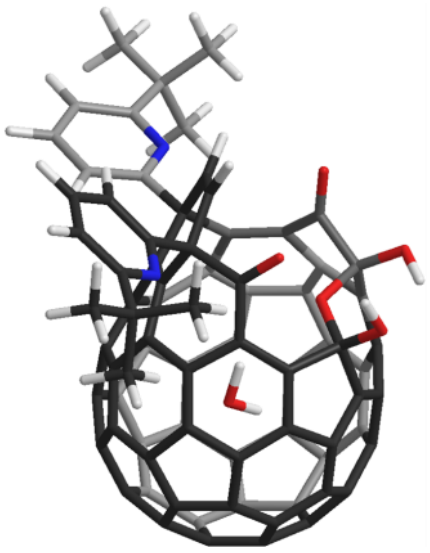
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.959973	1.177908	-3.334103
2	6	0	1.519053	1.345962	-3.333373
3	6	0	0.704855	0.248204	-3.505630
4	6	0	1.275466	-1.074673	-3.664966
5	6	0	2.651507	-1.246251	-3.622746
6	6	0	3.513294	-0.091306	-3.452803
7	6	0	1.162191	2.363662	-2.363539
8	6	0	-0.501152	0.142782	-2.728793
9	6	0	0.402088	-1.995540	-2.978568
10	6	0	3.214090	-2.345897	-2.863287
11	6	0	4.615593	-0.480514	-2.594569
12	6	0	3.508838	2.127884	-2.394903
13	6	0	2.370479	-3.225422	-2.194955
14	6	0	0.933784	-3.048557	-2.259712
15	6	0	2.692658	-3.653723	-0.851050
16	6	0	0.363806	-3.372107	-0.970155
17	6	0	0.007692	2.261802	-1.571817
18	6	0	-0.711996	-1.255949	-2.425944
19	6	0	1.454947	-3.738206	-0.108240
20	6	0	-1.338276	-1.618316	-1.243874
21	6	0	-0.875274	1.117926	-1.806789
22	6	0	4.420201	-1.867893	-2.215953
23	6	0	5.127715	0.424572	-1.675039
24	6	0	0.041632	2.797704	-0.203370
25	6	0	4.580511	1.764183	-1.585798
26	6	0	2.408785	2.884489	-1.836695
27	6	0	5.452380	-0.010179	-0.330820
28	6	0	4.605578	2.170697	-0.198549
29	6	0	2.460986	3.313532	-0.530588
30	6	0	-0.752354	-2.706160	-0.457230
31	6	0	4.722962	-2.278928	-0.921811
32	6	0	-1.824160	0.730975	-0.787162
33	6	0	5.114713	1.059162	0.584337
34	6	0	3.588882	2.957829	0.310394
35	6	0	1.262750	3.288725	0.268297
36	6	0	1.670279	3.004825	1.616622
37	6	0	-0.957265	2.350452	0.762546
38	6	0	-2.082138	-0.594799	-0.540627
39	6	0	-2.102538	-1.953260	1.549556
40	6	0	3.066486	2.707116	1.632308
41	6	0	3.493017	1.593450	2.349975
42	6	0	2.566490	0.777924	3.101386
43	6	0	4.534730	0.761265	1.808918
44	6	0	3.831763	-3.178280	-0.223060
45	6	0	-1.124530	1.350197	3.230948
46	6	0	5.237832	-1.325593	0.042328
47	6	0	4.640250	-1.625216	1.329471
48	6	0	-0.567993	2.139164	2.069110
49	6	0	-0.875462	-2.568952	0.974871
50	6	0	0.248395	-2.744487	1.753266
51	6	0	0.815602	2.305788	2.435033
52	6	0	1.276651	1.225406	3.260870
53	6	0	4.250062	-0.603871	2.183138

54	6	0	2.999206	-0.645723	2.931408
55	6	0	0.061938	0.427719	3.680771
56	6	0	3.783195	-2.758913	1.168953
57	6	0	1.416736	-3.326151	1.215059
58	6	0	0.640447	-1.875397	2.968294
59	6	0	2.589089	-2.789759	1.868059
60	6	0	2.183341	-1.755642	2.786534
61	6	0	-2.270146	1.839973	0.152625
62	6	0	-2.954872	-1.065506	0.604605
63	6	0	-3.531271	0.069898	1.401122
64	6	0	-3.235605	1.347513	1.195885
65	6	0	-4.074624	-1.949908	0.031794
66	6	0	-2.972314	2.969088	-0.615109
67	8	0	-2.421579	-2.144066	2.702347
68	8	0	-2.164463	1.424694	3.816613
69	7	0	-2.720991	4.205025	-0.205088
70	6	0	-3.339390	5.238235	-0.797119
71	6	0	-4.256057	5.036420	-1.829452
72	6	0	-4.528354	3.735422	-2.246399
73	6	0	-3.879486	2.673906	-1.634691
74	6	0	-5.288625	-1.397761	-0.374849
75	6	0	-6.236658	-2.257885	-0.911981
76	6	0	-5.947254	-3.614380	-1.026133
77	6	0	-4.701035	-4.080038	-0.601387
78	7	0	-3.791356	-3.242705	-0.084373
79	8	0	-0.060191	-0.664844	2.762837
80	8	0	-0.077561	0.106249	5.003254
81	8	0	0.332547	-2.441446	4.204856
82	6	0	-2.945589	6.611434	-0.260937
83	6	0	-4.256520	-5.536816	-0.695852
84	6	0	-3.800819	-6.000933	0.696125
85	6	0	-3.068256	-5.607038	-1.668774
86	6	0	-5.376736	-6.450657	-1.196511
87	6	0	-3.693965	7.744635	-0.965306
88	6	0	-1.433157	6.787230	-0.474471
89	6	0	-3.252863	6.652418	1.243888
90	1	0	-4.192640	-0.214820	2.213932
91	1	0	-3.653648	2.113334	1.842727
92	1	0	-4.751346	5.874556	-2.303630
93	1	0	-5.240808	3.556862	-3.045931
94	1	0	-4.057154	1.644726	-1.931293
95	1	0	-5.474302	-0.334919	-0.262546
96	1	0	-7.198735	-1.876356	-1.239936
97	1	0	-6.681667	-4.295337	-1.437838
98	1	0	0.410156	-0.709732	5.188230
99	1	0	-0.630166	-2.591192	4.185913
100	1	0	-3.428045	-7.028755	0.643136
101	1	0	-4.631057	-5.972705	1.408991
102	1	0	-3.004350	-5.354175	1.071660
103	1	0	-2.700457	-6.635825	-1.737978
104	1	0	-2.252760	-4.966835	-1.322202
105	1	0	-3.363083	-5.279525	-2.671031
106	1	0	-5.017658	-7.483345	-1.225990
107	1	0	-5.696040	-6.182999	-2.209056
108	1	0	-6.249411	-6.418954	-0.535946
109	1	0	-3.377452	8.704695	-0.547495
110	1	0	-4.776991	7.661401	-0.826296
111	1	0	-3.481033	7.763672	-2.039196
112	1	0	-1.104162	7.745509	-0.059772
113	1	0	-1.184950	6.771336	-1.540744
114	1	0	-0.884034	5.981215	0.018710
115	1	0	-2.930287	7.610092	1.664856
116	1	0	-2.728843	5.845321	1.760507
117	1	0	-4.326542	6.541172	1.426805
118	8	0	1.838641	-0.029281	0.100389
119	1	0	1.368516	-0.043351	-0.745065
120	1	0	1.129125	-0.037125	0.762319

The total electronic energy was calculated to be –3702.2258469 Hartree.

Table S17. Optimized structure of H_2O@**1B** (M06-2X/6-31G(d,p))



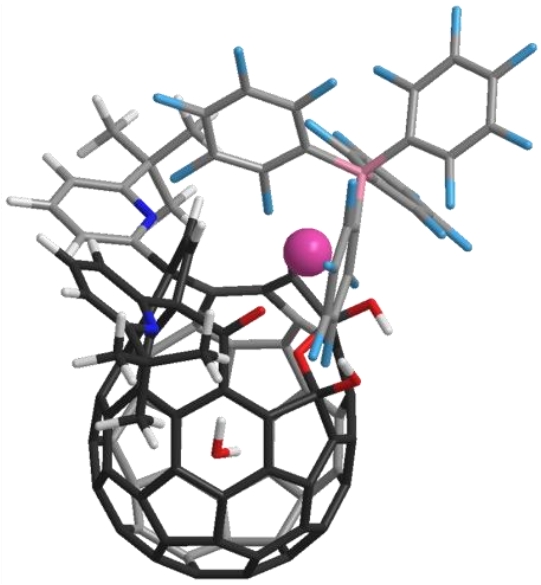
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.043174	1.304745	-3.265340
2	6	0	1.599881	1.433838	-3.309510
3	6	0	0.825804	0.314592	-3.512044
4	6	0	1.436967	-0.988862	-3.664223
5	6	0	2.812907	-1.123334	-3.583678
6	6	0	3.634578	0.053080	-3.377091
7	6	0	1.184365	2.429105	-2.341535
8	6	0	-0.398192	0.167034	-2.775037
9	6	0	0.570375	-1.940154	-3.014348
10	6	0	3.381766	-2.213717	-2.817430
11	6	0	4.719326	-0.313296	-2.487868
12	6	0	3.536896	2.259034	-2.300435
13	6	0	2.544040	-3.121910	-2.183650
14	6	0	1.106894	-2.985693	-2.291463
15	6	0	2.836575	-3.555204	-0.835927
16	6	0	0.505823	-3.341411	-1.025804
17	6	0	0.010966	2.285054	-1.586636
18	6	0	-0.578569	-1.237655	-2.490559
19	6	0	1.579132	-3.684930	-0.133772
20	6	0	-1.232841	-1.630589	-1.334708
21	6	0	-0.829494	1.120687	-1.858856
22	6	0	4.552356	-1.709566	-2.128581
23	6	0	5.183873	0.597045	-1.547993
24	6	0	-0.013436	2.808020	-0.212483
25	6	0	4.596591	1.920742	-1.463733
26	6	0	2.398516	2.977885	-1.769487
27	6	0	5.480288	0.157116	-0.198117
28	6	0	4.568039	2.315989	-0.072276
29	6	0	2.398655	3.400432	-0.459421

30	6	0	-0.644270	-2.712327	-0.541465	77	6	0	-4.608355	-4.226829	-0.637012
31	6	0	4.830546	-2.128297	-0.831426	78	7	0	-3.733063	-3.361461	-0.104842
32	6	0	-1.798535	0.699154	-0.873791	79	8	0	-0.111002	-0.685708	2.719581
33	6	0	5.083593	1.209101	0.716588	80	8	0	-0.211300	0.066217	4.963888
34	6	0	3.511167	3.068071	0.412838	81	8	0	0.291575	-2.464209	4.154888
35	6	0	1.177294	3.331583	0.301870	82	6	0	-3.273658	6.511343	-0.092489
36	6	0	1.550276	3.047782	1.660841	83	6	0	-4.215333	-5.695483	-0.508012
37	6	0	-1.029936	2.325109	0.718831	84	6	0	-4.047554	-6.016907	0.985880
38	6	0	-2.024099	-0.635044	-0.644274	85	6	0	-2.871751	-5.899902	-1.225565
39	6	0	-2.071946	-2.011514	1.433588	86	6	0	-5.264209	-6.628968	-1.115061
40	6	0	2.954826	2.790086	1.717018	87	6	0	-4.014267	7.649135	-0.797598
41	6	0	3.390646	1.680988	2.438866	88	6	0	-1.762679	6.793522	-0.112684
42	6	0	2.462273	0.830213	3.150328	89	6	0	-3.752281	6.415171	1.364635
43	6	0	4.473810	0.883330	1.922397	90	1	0	-4.248933	-0.343890	2.029784
44	6	0	3.944246	-3.059497	-0.169580	91	1	0	-3.762602	2.005202	1.697122
45	6	0	-1.246202	1.293489	3.168738	92	1	0	-4.804790	5.827001	-2.365451
46	6	0	5.288858	-1.168884	0.156476	93	1	0	-5.055515	3.547189	-3.317201
47	6	0	4.658395	-1.497584	1.421766	94	1	0	-3.862387	1.632357	-2.225634
48	6	0	-0.675652	2.113182	2.035040	95	1	0	-5.292366	-0.450178	-0.744192
49	6	0	-0.814624	-2.593201	0.888008	96	1	0	-6.944039	-2.043258	-1.768773
50	6	0	0.288507	-2.746531	1.699599	97	1	0	-6.485212	-4.481601	-1.674715
51	6	0	0.689910	2.316122	2.445795	98	1	0	0.264467	-0.757377	5.147278
52	6	0	1.155099	1.237843	3.271214	99	1	0	-0.664446	-2.647153	4.102239
53	6	0	4.212668	-0.494693	2.272320	100	1	0	-3.714140	-7.052132	1.110702
54	6	0	2.937888	-0.578754	2.976666	101	1	0	-4.995511	-5.894976	1.519653
55	6	0	-0.048106	0.398910	3.646291	102	1	0	-3.310309	-5.349880	1.439317
56	6	0	3.840153	-2.654774	1.223765	103	1	0	-2.542226	-6.937918	-1.114430
57	6	0	1.488218	-3.291701	1.192432	104	1	0	-2.108670	-5.241696	-0.802444
58	6	0	0.616521	-1.875896	2.931675	105	1	0	-2.961415	-5.680597	-2.294529
59	6	0	2.625141	-2.726355	1.883975	106	1	0	-4.942595	-7.667187	-0.992308
60	6	0	2.159611	-1.710426	2.794810	107	1	0	-5.396594	-6.446253	-2.186552
61	6	0	-2.307630	1.784275	0.060767	108	1	0	-6.235310	-6.520536	-0.620968
62	6	0	-2.917850	-1.142577	0.467772	109	1	0	-3.813310	8.591485	-0.279866
63	6	0	-3.562750	-0.032224	1.248088	110	1	0	-5.097667	7.490347	-0.791315
64	6	0	-3.297004	1.255367	1.063909	111	1	0	-3.685079	7.763576	-1.835618
65	6	0	-3.986622	-2.059165	-0.146036	112	1	0	-1.549468	7.733111	0.407168
66	6	0	-3.009069	2.912218	-0.708485	113	1	0	-1.395002	6.879200	-1.140440
67	8	0	-2.415489	-2.215075	2.577084	114	1	0	-1.218824	5.984153	0.380654
68	8	0	-2.306364	1.330720	3.719905	115	1	0	-3.552832	7.356218	1.887238
69	7	0	-2.886640	4.126961	-0.188111	116	1	0	-3.231952	5.606596	1.882712
70	6	0	-3.511627	5.162890	-0.766570	117	1	0	-4.828544	6.219554	1.410578
71	6	0	-4.304080	4.986271	-1.901672	118	8	0	1.847561	-0.398904	-0.494444
72	6	0	-4.442635	3.707427	-2.435314	119	1	0	2.573097	0.072220	-0.058492
73	6	0	-3.787335	2.642325	-1.835453	120	1	0	1.094319	-0.272762	0.102749
74	6	0	-5.129852	-1.523117	-0.738441						
75	6	0	-6.036916	-2.410696	-1.298696						
76	6	0	-5.780419	-3.778914	-1.247955						

The total electronic energy was calculated to be –3702.2260099 Hartree.

Table S18. Optimized structure of $[Li^{+}\subset(H_2O@\mathbf{1})][B(C_6F_5)_4]^{-}$ (M06-2X/6-31G(d,p))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.693126	0.141092	0.388734
2	6	0	-6.790993	0.659781	1.398121
3	6	0	-6.145075	-0.213792	2.243299
4	6	0	-6.340572	-1.642990	2.119620
5	6	0	-7.168278	-2.144750	1.129644
6	6	0	-7.860445	-1.229628	0.243783
7	6	0	-6.073161	1.793967	0.849960
8	6	0	-4.774264	0.036180	2.589563
9	6	0	-5.069608	-2.267782	2.392018
10	6	0	-6.743496	-3.292619	0.354425
11	6	0	-7.871151	-1.817684	-1.081441
12	6	0	-7.576374	0.986344	-0.776984
13	6	0	-5.515252	-3.885745	0.615241
14	6	0	-4.660109	-3.363157	1.660315
15	6	0	-4.661654	-4.287132	-0.479398
16	6	0	-3.281800	-3.439447	1.224596
17	6	0	-4.724617	2.033314	1.147892
18	6	0	-4.107813	-1.240413	2.712657
19	6	0	-3.294999	-4.008683	-0.095025
20	6	0	-2.762716	-1.349973	2.400708
21	6	0	-4.076972	1.134293	2.098940
22	6	0	-7.167921	-3.084724	-1.015197
23	6	0	-7.746052	-1.008203	-2.202129
24	6	0	-3.865759	2.631390	0.112710
25	6	0	-7.615386	0.428575	-2.051381
26	6	0	-6.614070	2.023862	-0.475250
27	6	0	-6.892799	-1.417990	-3.300357
28	6	0	-6.715038	0.912332	-3.076419
29	6	0	-5.795855	2.519868	-1.465942
30	6	0	-2.325418	-2.480907	1.577416
31	6	0	-6.345348	-3.473702	-2.066386
32	6	0	-2.636826	1.071978	2.138083
33	6	0	-6.241562	-0.236751	-3.830523
34	6	0	-5.848464	1.958235	-2.803370
35	6	0	-4.424822	2.836568	-1.152954
36	6	0	-3.651205	2.563650	-2.334644
37	6	0	-2.415688	2.521104	0.231529
38	6	0	-1.997861	-0.126487	2.332945
39	6	0	-0.194048	-1.214153	1.032331
40	6	0	-4.492768	1.933053	-3.303857
41	6	0	-4.013548	0.799883	-3.955629
42	6	0	-2.684647	0.289690	-3.697358
43	6	0	-4.909138	-0.298067	-4.219217
44	6	0	-5.060784	-4.074053	-1.788030
45	6	0	-0.349679	1.684200	-1.149704
46	6	0	-6.193767	-2.611331	-3.224240
47	6	0	-4.805685	-2.666746	-3.641679
48	6	0	-1.674385	2.313913	-0.921918
49	6	0	-1.233677	-2.215591	0.658587
50	6	0	-1.360480	-2.641608	-0.653867
51	6	0	-2.344140	2.158523	-2.195001
52	6	0	-1.815630	1.060024	-2.959205
53	6	0	-4.156059	-1.523917	-4.088456
54	6	0	-2.787457	-1.206211	-3.702564
55	6	0	-0.569590	0.595152	-2.244723
56	6	0	-4.115673	-3.565350	-2.766743
57	6	0	-2.394728	-3.528355	-1.033187
58	6	0	-0.948499	-1.829255	-1.904884
59	6	0	-2.820277	-3.258497	-2.391267
60	6	0	-2.127944	-2.092999	-2.870273
61	6	0	-1.911795	2.325387	1.672403
62	6	0	-0.498584	-0.283980	2.232924
63	6	0	0.200966	1.038034	2.076329
64	6	0	-0.420593	2.180935	1.808460
65	6	0	0.053406	-1.012406	3.468310
66	6	0	-2.313046	3.547977	2.512809
67	8	0	0.849175	-1.119005	0.406503
68	8	0	0.741767	1.844410	-0.651529
69	7	0	-2.402807	4.696876	1.855991
70	6	0	-2.705817	5.820108	2.524405
71	6	0	-2.913323	5.802730	3.904826
72	6	0	-2.798400	4.597088	4.591739
73	6	0	-2.491825	3.439483	3.891697
74	6	0	0.231789	-0.341678	4.675811
75	6	0	0.774448	-1.063807	5.728719
76	6	0	1.109957	-2.403016	5.544784
77	6	0	0.885663	-2.997457	4.301645
78	7	0	0.358096	-2.291756	3.290761
79	8	0	-0.927388	-0.498770	-1.424010
80	8	0	0.613547	0.431795	-2.926459
81	8	0	0.237203	-2.202720	-2.517494
82	6	0	-2.807537	7.073926	1.660914
83	6	0	1.195639	-4.454267	3.974080
84	6	0	2.095804	-4.501880	2.728937
85	6	0	-0.133635	-5.161396	3.661516
86	6	0	1.893160	-5.166953	5.134235
87	6	0	-3.169459	8.312795	2.482305
88	6	0	-3.888765	6.833703	0.594517
89	6	0	-1.453102	7.295737	0.969307
90	3	0	1.972941	0.297268	-0.536299
91	6	0	2.718297	2.710834	-3.088877

92	6	0	3.073299	3.127985	-1.819883	131	9	0	4.488167	-0.410948	-3.276489
93	6	0	3.894145	2.320830	-1.033335	132	9	0	2.843471	1.074464	-4.777374
94	6	0	4.387369	1.088581	-1.456603	133	9	0	1.854511	3.418911	-3.812359
95	6	0	4.043998	0.747435	-2.767838	134	9	0	2.561813	4.254117	-1.324236
96	6	0	3.220690	1.511391	-3.576491	135	9	0	4.150475	2.790516	0.196447
97	6	0	8.642038	-0.305629	-2.956917	136	1	0	1.279895	1.020875	2.183553
98	6	0	7.475857	-0.589635	-2.252191	137	1	0	0.155324	3.091882	1.668405
99	6	0	6.849036	0.329965	-1.421894	138	1	0	-3.159710	6.711603	4.439127
100	6	0	7.454155	1.582926	-1.367877	139	1	0	-2.952006	4.564171	5.665850
101	6	0	8.614548	1.910683	-2.049276	140	1	0	-2.400216	2.478011	4.387034
102	6	0	9.214605	0.951360	-2.854597	141	1	0	-0.020531	0.709890	4.766170
103	6	0	4.951470	-1.464375	-0.565156	142	1	0	0.946638	-0.586590	6.688281
104	6	0	5.804431	-2.385087	0.048403	143	1	0	1.547316	-2.969464	6.357531
105	6	0	5.453282	-3.691937	0.353319	144	1	0	0.636930	-0.445567	-3.343410
106	6	0	4.172513	-4.144204	0.055290	145	1	0	0.916142	-2.330161	-1.832335
107	6	0	3.285589	-3.270930	-0.544387	146	1	0	2.313910	-5.539969	2.463509
108	6	0	3.704705	-1.984948	-0.852044	147	1	0	3.047251	-3.990273	2.912712
109	6	0	4.229145	0.695664	3.065443	148	1	0	1.603697	-4.020591	1.878901
110	6	0	5.396998	0.902702	3.785301	149	1	0	0.053765	-6.202744	3.381354
111	6	0	6.608559	0.894119	3.112552	150	1	0	-0.645256	-4.662326	2.833626
112	6	0	6.642808	0.681317	1.735525	151	1	0	-0.796385	-5.153669	4.532943
113	6	0	5.499698	0.489263	0.965886	152	1	0	2.108189	-6.201058	4.851029
114	6	0	4.325607	0.496792	1.701733	153	1	0	1.265051	-5.192872	6.030616
115	5	0	5.435773	0.115377	-0.638116	154	1	0	2.843447	-4.685985	5.387926
116	9	0	3.129543	0.287125	1.061755	155	1	0	-3.232289	9.182112	1.821775
117	9	0	3.041104	0.686480	3.682887	156	1	0	-2.412282	8.527646	3.243404
118	9	0	5.350748	1.097929	5.101171	157	1	0	-4.139636	8.200292	2.977373
119	9	0	7.737043	1.079017	3.793662	158	1	0	-3.956686	7.700607	-0.070236
120	9	0	7.858734	0.660727	1.186278	159	1	0	-4.868383	6.678594	1.058230
121	9	0	7.036309	-1.998766	0.395434	160	1	0	-3.645016	5.950717	-0.001509
122	9	0	6.318041	-4.512617	0.943644	161	1	0	-1.509675	8.164736	0.306286
123	9	0	3.802581	-5.385855	0.358479	162	1	0	-1.179182	6.419392	0.377621
124	9	0	2.028615	-3.657833	-0.821226	163	1	0	-0.663316	7.477383	1.705074
125	9	0	2.740453	-1.224561	-1.472884	164	8	0	-4.656998	-1.085158	-0.606336
126	9	0	6.901926	2.542379	-0.605665	165	1	0	-3.764960	-0.770288	-0.397984
127	9	0	9.154553	3.126164	-1.948562	166	1	0	-4.947114	-0.509901	-1.329678
128	9	0	10.330800	1.239210	-3.521603						
129	9	0	9.206872	-1.230523	-3.734771						
130	9	0	6.977140	-1.823941	-2.420189						

The total electronic energy was calculated to be –6644.968403 Hartree.

10. TD DFT Calculations

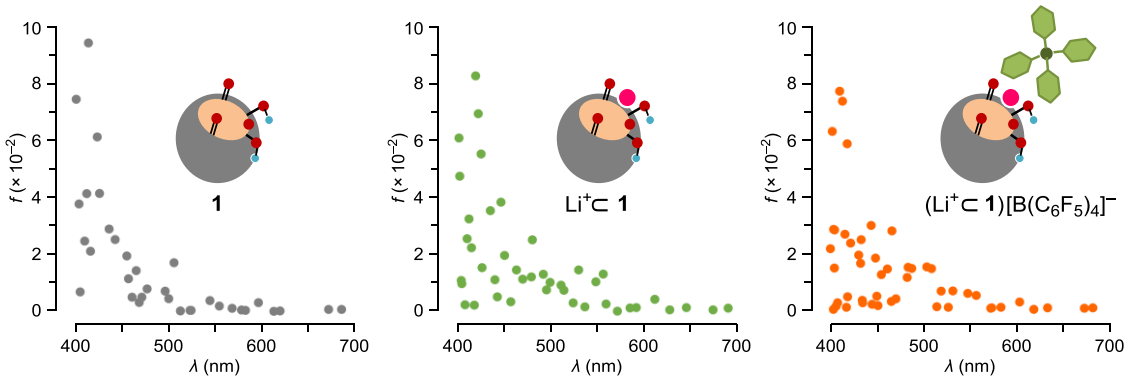


Figure S11. Plots of oscillator strengths for **1**, $Li^+ \subset$ **1**, and $(Li^+ \subset \mathbf{1})[B(C_6F_5)_4]^-$. The transition energies were calibrated with a factor of 0.72 (TD-CAM-B3LYP/6-31G(d)//B3LYP/6-31G(d)).

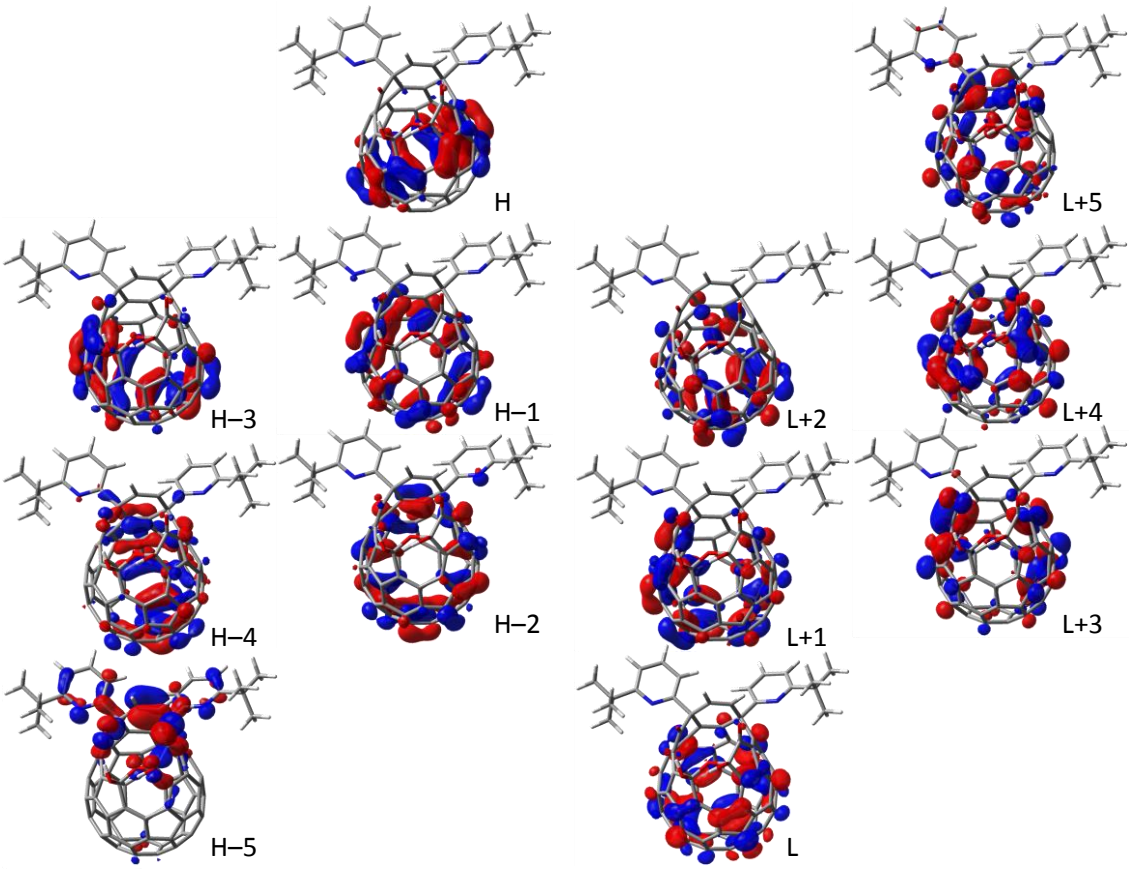


Figure S12. Pictorial representation of the Kohn-Sham HOMOs and LUMOs for **1** (B3LYP/6-31G(d)).

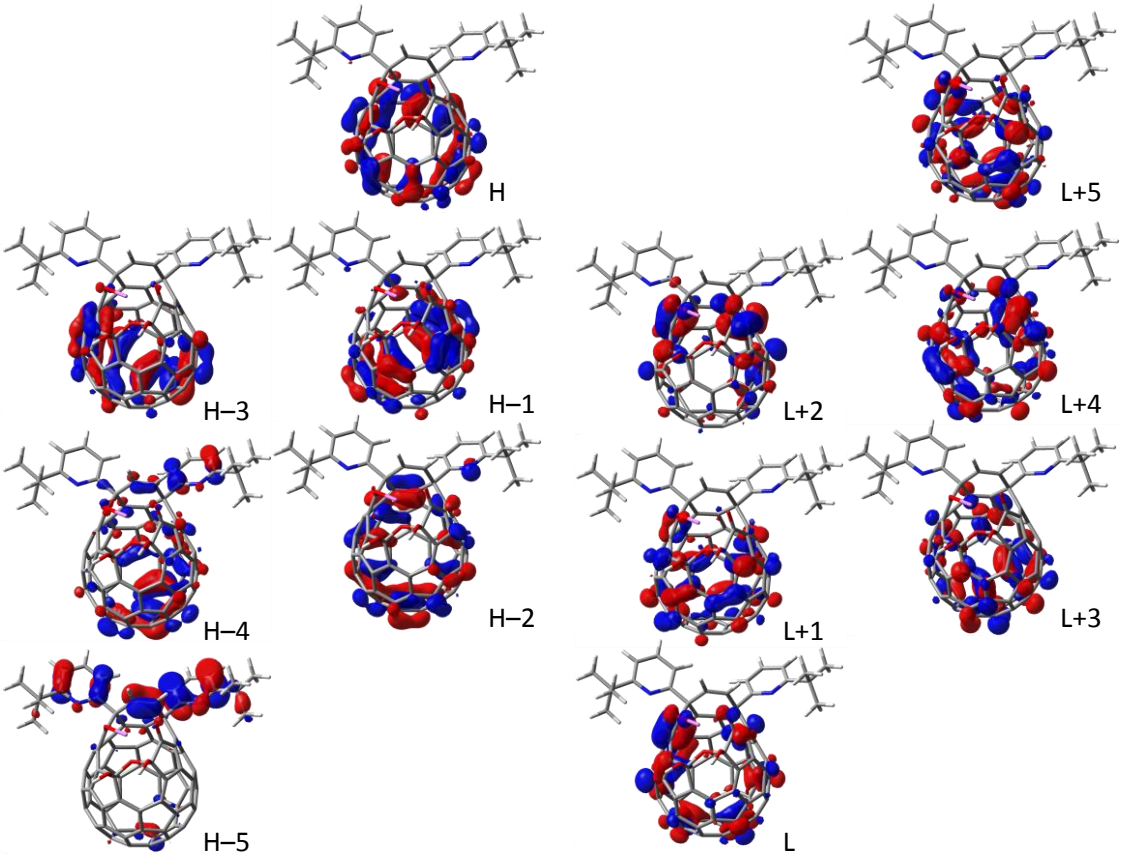


Figure S13. Pictorial representation of the Kohn-Sham HOMOs and LUMOs for $Li^{+}\subset$**1** (B3LYP/6-31G(d)).

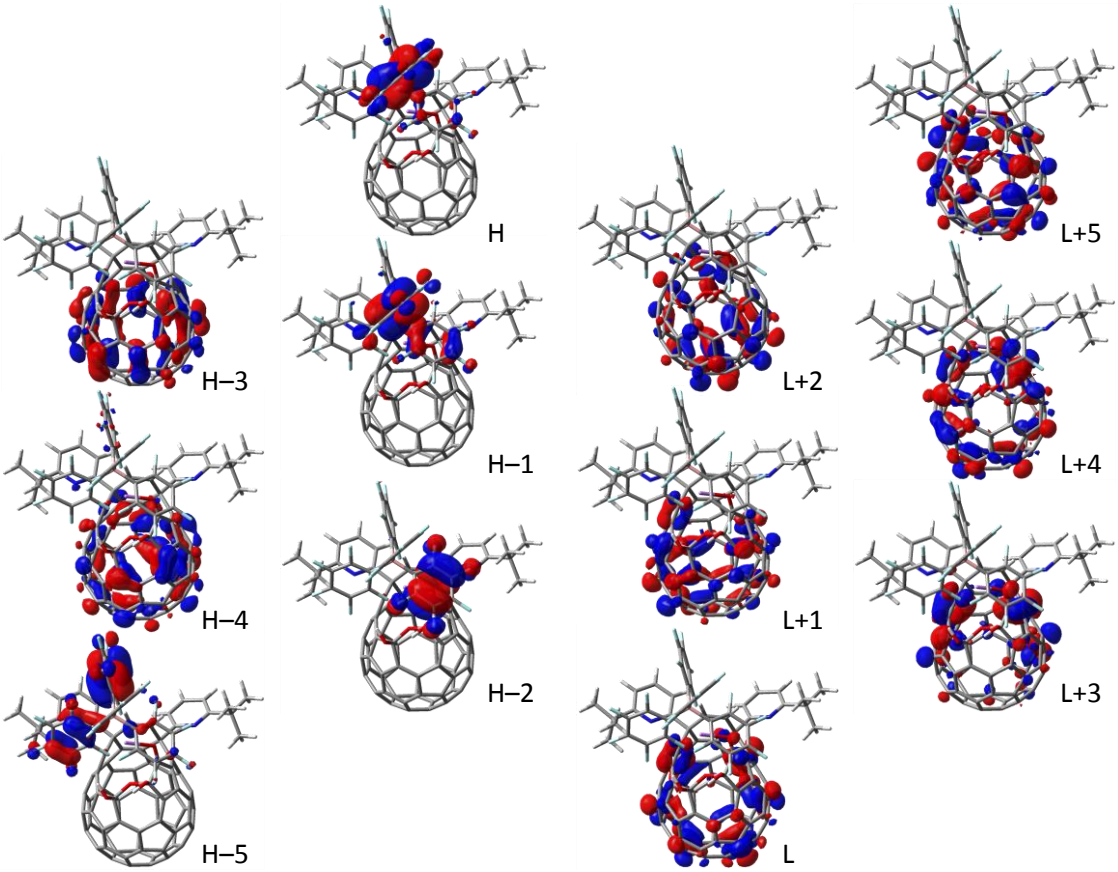
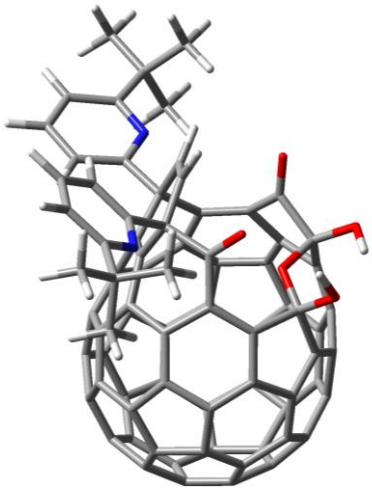


Figure S14. Pictorial representation of the Kohn-Sham HOMOs and LUMOs for $(Li^{+}\subset\mathbf{1})[B(C_6F_5)_4]^{-}$ (B3LYP/6-31G(d)).

Table S19. Optimized structure of **1** (B3LYP/6-31G(d))



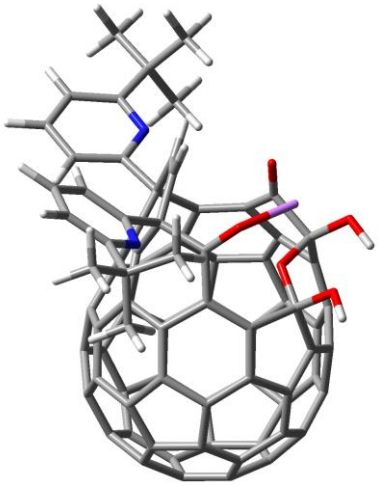
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.137252	1.277047	-3.309074
2	6	0	1.689596	1.387658	-3.363681
3	6	0	0.922620	0.251362	-3.555012
4	6	0	1.551390	-1.051137	-3.680232
5	6	0	2.937851	-1.168614	-3.584502
6	6	0	3.748080	0.022496	-3.395403
7	6	0	1.255769	2.396677	-2.414577
8	6	0	-0.307115	0.103012	-2.822838
9	6	0	0.688437	-2.001027	-3.016689
10	6	0	3.514549	-2.239958	-2.790813
11	6	0	4.832282	-0.314437	-2.489232
12	6	0	3.614248	2.257757	-2.358557
13	6	0	2.675735	-3.150680	-2.140841
14	6	0	1.234638	-3.031828	-2.262732
15	6	0	2.962705	-3.552188	-0.777914
16	6	0	0.627774	-3.362543	-0.990453
17	6	0	0.072382	2.247500	-1.656612
18	6	0	-0.474491	-1.300238	-2.515806
19	6	0	1.699464	-3.675390	-0.080198
20	6	0	-1.138766	-1.677358	-1.350122
21	6	0	-0.759749	1.071605	-1.916785
22	6	0	4.677107	-1.707504	-2.102734
23	6	0	5.281276	0.624673	-1.557568
24	6	0	0.030167	2.799397	-0.291714
25	6	0	4.677890	1.945511	-1.502845
26	6	0	2.461748	2.973048	-1.846489
27	6	0	5.574987	0.214716	-0.195170
28	6	0	4.636812	2.367720	-0.117695
29	6	0	2.447583	3.419613	-0.537236
30	6	0	-0.538500	-2.730100	-0.524537
31	6	0	4.951001	-2.098089	-0.786534
32	6	0	-1.743624	0.659480	-0.939303
33	6	0	5.162690	1.282513	0.696570
34	6	0	3.562008	3.120089	0.349655
35	6	0	1.222090	3.349772	0.219721
36	6	0	1.592399	3.099217	1.586209
37	6	0	-0.990240	2.329491	0.643955
38	6	0	-1.963661	-0.683206	-0.695487
39	6	0	-2.018790	-2.052256	1.408944
40	6	0	3.002788	2.862247	1.657494
41	6	0	3.451111	1.767660	2.407932
42	6	0	2.525836	0.918900	3.131963
43	6	0	4.545583	0.971811	1.911601
44	6	0	4.066857	-3.025216	-0.110286
45	6	0	-1.201628	1.363551	3.133375
46	6	0	5.395479	-1.113424	0.186765
47	6	0	4.758937	-1.423497	1.456047
48	6	0	-0.632690	2.146700	1.974255
49	6	0	-0.727494	-2.588724	0.905096
50	6	0	0.379004	-2.713013	1.735697
51	6	0	0.732354	2.366313	2.380678
52	6	0	1.205467	1.312613	3.233904
53	6	0	4.296470	-0.402990	2.287594
54	6	0	3.015779	-0.485829	2.989639
55	6	0	0.009825	0.479558	3.645708
56	6	0	3.948532	-2.592568	1.275900
57	6	0	1.591460	-3.248828	1.243858
58	6	0	0.696269	-1.820073	2.964368
59	6	0	2.721190	-2.660373	1.932010
60	6	0	2.244613	-1.636758	2.831594
61	6	0	-2.270249	1.757579	-0.014078
62	6	0	-2.870343	-1.196007	0.411930
63	6	0	-3.523983	-0.074612	1.177518
64	6	0	-3.258930	1.216626	0.990747
65	6	0	-3.953183	-2.117393	-0.199434
66	6	0	-3.008021	2.876708	-0.785609
67	8	0	-2.397494	-2.271496	2.546469
68	8	0	-2.270557	1.421693	3.681673
69	7	0	-2.981865	4.081830	-0.214337
70	6	0	-3.655917	5.105906	-0.769450
71	6	0	-4.395941	4.926495	-1.944667
72	6	0	-4.432291	3.663998	-2.536539
73	6	0	-3.732247	2.612880	-1.953632
74	6	0	-5.077864	-1.572939	-0.828945
75	6	0	-6.009870	-2.453915	-1.365787
76	6	0	-5.800408	-3.829108	-1.254236
77	6	0	-4.648624	-4.294002	-0.608760
78	7	0	-3.746499	-3.431072	-0.103326
79	8	0	-0.072439	-0.650401	2.760078
80	8	0	-0.110668	0.179425	4.986862
81	8	0	0.377656	-2.416241	4.208478
82	6	0	-3.540160	6.445439	-0.027858
83	6	0	-4.317888	-5.780406	-0.413007
84	6	0	-4.160425	-6.050911	1.101227
85	6	0	-2.983224	-6.087278	-1.130326
86	6	0	-5.412985	-6.703154	-0.976110
87	6	0	-4.370286	7.557509	-0.692492
88	6	0	-2.052125	6.865836	-0.011387
89	6	0	-4.029453	6.249470	1.425266
90	1	0	-4.220104	-0.378830	1.952735
91	1	0	-3.742728	1.962794	1.612357
92	1	0	-4.937115	5.750739	-2.393389
93	1	0	-5.003322	3.503913	-3.447556
94	1	0	-3.740931	1.620432	-2.391780
95	1	0	-5.214741	-0.497915	-0.881824

96	1	0	-6.899297	-2.075654	-1.863186
97	1	0	-6.527117	-4.521553	-1.661432
98	1	0	0.188916	-0.741147	5.119447
99	1	0	-0.570356	-2.652289	4.134630
100	1	0	-3.864692	-7.093310	1.269934
101	1	0	-5.103649	-5.876499	1.632606
102	1	0	-3.401355	-5.395882	1.536590
103	1	0	-2.695431	-7.131944	-0.962372
104	1	0	-2.182877	-5.442533	-0.757622
105	1	0	-3.071352	-5.930610	-2.212245
106	1	0	-5.135614	-7.749106	-0.804631
107	1	0	-5.545310	-6.572375	-2.056683
108	1	0	-6.380235	-6.535627	-0.487794
109	1	0	-4.259953	8.487880	-0.124587
110	1	0	-5.438727	7.312218	-0.716915
111	1	0	-4.040332	7.759289	-1.718474
112	1	0	-1.926653	7.792337	0.561534
113	1	0	-1.679823	7.043049	-1.027678
114	1	0	-1.436295	6.086703	0.445993
115	1	0	-3.910240	7.180390	1.992195
116	1	0	-3.457768	5.461922	1.922884
117	1	0	-5.089867	5.970967	1.451027

The total electronic energy was calculated to be –3627.0049709 Hartree.

Table S20. Optimized structure of $Li^{+}\subset$**1** (B3LYP/6-31G(d))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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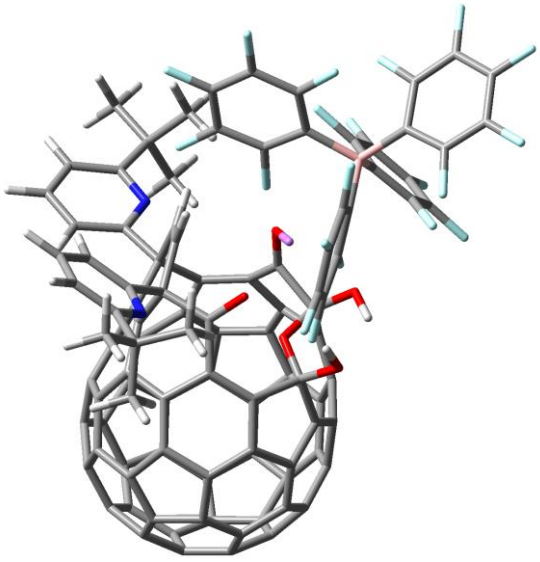
2	6	0	1.987793	1.203456	-3.333652
3	6	0	1.063147	0.204048	-3.581208
4	6	0	1.487681	-1.177445	-3.721632
5	6	0	2.834242	-1.509470	-3.584890
6	6	0	3.811176	-0.462411	-3.340720
7	6	0	1.682148	2.241873	-2.365780
8	6	0	-0.199038	0.232785	-2.893729
9	6	0	0.468706	-1.995509	-3.105781
10	6	0	3.209940	-2.672762	-2.800788
11	6	0	4.800212	-0.983024	-2.412890
12	6	0	3.987885	1.741260	-2.246117
13	6	0	2.219843	-3.455153	-2.198748
14	6	0	0.819640	-3.111124	-2.358226
15	6	0	2.398179	-3.922140	-0.839444
16	6	0	0.129262	-3.360967	-1.108345
17	6	0	0.465954	2.260189	-1.649744
18	6	0	-0.587163	-1.134235	-2.624166
19	6	0	1.109794	-3.856966	-0.180028
20	6	0	-1.340355	-1.424955	-1.490762
21	6	0	-0.525995	1.239083	-1.975919
22	6	0	4.419562	-2.342975	-2.068087
23	6	0	5.358421	-0.146121	-1.444321
24	6	0	0.460555	2.772285	-0.265624
25	6	0	4.963142	1.250066	-1.370445
26	6	0	2.941632	2.609584	-1.744404
27	6	0	5.544597	-0.627643	-0.087402
28	6	0	4.942527	1.642263	0.023753
29	6	0	2.953169	3.024377	-0.424653
30	6	0	-0.937295	-2.561774	-0.657278
31	6	0	4.592170	-2.802526	-0.757443
32	6	0	-1.597021	0.967847	-1.046036
33	6	0	5.273908	0.471019	0.821472
34	6	0	3.982258	2.540357	0.482348
35	6	0	1.707382	3.117168	0.296266
36	6	0	1.994537	2.790390	1.667648
37	6	0	-0.654987	2.452234	0.622669
38	6	0	-2.030986	-0.328408	-0.852932
39	6	0	-2.351217	-1.661821	1.222482
40	6	0	3.351541	2.339450	1.767150
41	6	0	3.615930	1.178166	2.502494
42	6	0	2.551769	0.465626	3.178698
43	6	0	4.588645	0.233775	2.013753
44	6	0	3.552928	-3.592915	-0.131929
45	6	0	-1.069134	1.400771	2.997479
46	6	0	5.153806	-1.920846	0.253571
47	6	0	4.438423	-2.155311	1.496477
48	6	0	-0.366971	2.192845	1.970064
49	6	0	-1.159182	-2.425570	0.775645
50	6	0	-0.110774	-2.767650	1.642156
51	6	0	1.010564	2.189174	2.423967
52	6	0	1.312009	1.067504	3.274742
53	6	0	4.121545	-1.095176	2.346768
54	6	0	2.825396	-0.995291	3.011708
55	6	0	0.003357	0.427972	3.604644
56	6	0	3.460563	-3.177982	1.260868
57	6	0	1.021655	-3.463833	1.156744
58	6	0	0.339235	-1.974499	2.907054
59	6	0	2.219425	-3.073598	1.881067
60	6	0	1.890384	-2.005211	2.786978
61	6	0	-1.984182	2.111991	-0.108717
62	6	0	-3.056443	-0.727158	0.189521
63	6	0	-3.627614	0.478892	0.893733
64	6	0	-3.133956	1.712482	0.786957
65	6	0	-4.192997	-1.544555	-0.466601
66	6	0	-2.462233	3.377540	-0.861873
67	8	0	-2.756148	-1.710095	2.385730
68	8	0	-2.224947	1.297816	3.376162
69	7	0	-2.286512	4.518266	-0.192215
70	6	0	-2.726726	5.678719	-0.714400
71	6	0	-3.375829	5.700877	-1.956959
72	6	0	-3.569034	4.506051	-2.647875
73	6	0	-3.109761	3.312160	-2.097266
74	6	0	-5.131076	-0.924297	-1.295021
75	6	0	-6.126757	-1.723902	-1.846778
76	6	0	-6.154609	-3.087439	-1.553010
77	6	0	-5.177776	-3.631928	-0.709931

78	7	0	-4.211556	-2.848863	-0.187793
79	8	0	-0.264771	-0.710770	2.760683
80	8	0	-0.368343	0.153621	4.923828
81	8	0	-0.120800	-2.459692	4.170182
82	6	0	-2.471036	6.929300	0.137554
83	6	0	-5.122740	-5.112820	-0.311950
84	6	0	-5.192284	-5.210568	1.229867
85	6	0	-3.782512	-5.706841	-0.803931
86	6	0	-6.281755	-5.922922	-0.919116
87	6	0	-2.993547	8.211475	-0.534115
88	6	0	-0.948342	7.065554	0.368725
89	6	0	-3.180176	6.747701	1.499818
90	1	0	-4.477753	0.294822	1.543408
91	1	0	-3.584120	2.523051	1.351475
92	1	0	-3.729465	6.632230	-2.381569
93	1	0	-4.074018	4.507041	-3.609990
94	1	0	-3.244690	2.367417	-2.613214
95	1	0	-5.084062	0.142163	-1.490143
96	1	0	-6.880778	-1.290469	-2.498008
97	1	0	-6.931710	-3.712633	-1.975042
98	1	0	0.183444	-0.572397	5.270163
99	1	0	0.137313	-3.391807	4.272585
100	1	0	-5.106961	-6.257099	1.544158
101	1	0	-6.144940	-4.821628	1.608082
102	1	0	-4.383081	-4.639460	1.694029
103	1	0	-3.700813	-6.755840	-0.497109
104	1	0	-2.933900	-5.157218	-0.386639
105	1	0	-3.710374	-5.669121	-1.897306
106	1	0	-6.205816	-6.967620	-0.599717
107	1	0	-6.259494	-5.913967	-2.014988
108	1	0	-7.258561	-5.550157	-0.590254
109	1	0	-2.786828	9.072782	0.109810
110	1	0	-4.077037	8.178055	-0.697019
111	1	0	-2.505409	8.399294	-1.497591
112	1	0	-0.741930	7.923796	1.018300
113	1	0	-0.416663	7.222854	-0.577248
114	1	0	-0.545431	6.166171	0.842750
115	1	0	-2.980245	7.609887	2.146162
116	1	0	-2.825040	5.845358	2.005592
117	1	0	-4.266185	6.666053	1.373111
118	3	0	-2.167013	-0.727086	3.893133

The total electronic energy was calculated to be –3634.4337952 Hartree.

Table S21. Optimized structure of $(Li^{+}\subset\mathbf{1})[B(C_6F_5)_4]^{-}$ (B3LYP/6-31G(d))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.904130	0.310021	0.146101
2	6	0	-7.034749	0.741871	1.227249
3	6	0	-6.461315	-0.201769	2.062830
4	6	0	-6.699107	-1.618275	1.850198
5	6	0	-7.495940	-2.039404	0.787149
6	6	0	-8.114061	-1.052976	-0.082280
7	6	0	-6.249189	1.876805	0.776535
8	6	0	-5.100770	-0.021031	2.491501
9	6	0	-5.462940	-2.303096	2.151800
10	6	0	-7.067140	-3.160403	-0.030780
11	6	0	-8.078284	-1.569894	-1.439378
12	6	0	-7.700758	1.213052	-0.965602
13	6	0	-5.864096	-3.812251	0.258455
14	6	0	-5.046446	-3.375279	1.374396
15	6	0	-4.966222	-4.183220	-0.816327
16	6	0	-3.649157	-3.470376	0.999345
17	6	0	-4.898873	2.046084	1.152789
18	6	0	-4.485988	-1.328131	2.578182
19	6	0	-3.611081	-3.967638	-0.351310
20	6	0	-3.123573	-1.466314	2.325073
21	6	0	-4.332804	1.080466	2.092202
22	6	0	-7.417995	-2.864587	-1.408716
23	6	0	-7.865666	-0.701373	-2.512533
24	6	0	-3.963544	2.665412	0.194594
25	6	0	-7.694403	0.722286	-2.276631
26	6	0	-6.716480	2.196828	-0.560399
27	6	0	-6.972567	-1.083110	-3.592156
28	6	0	-6.728099	1.226383	-3.230935
29	6	0	-5.826151	2.712015	-1.485519
30	6	0	-2.679022	-2.556822	1.450902
31	6	0	-6.550556	-3.227290	-2.445349
32	6	0	-2.898681	0.967802	2.214709
33	6	0	-6.258074	0.102781	-4.026651
34	6	0	-5.835061	2.227543	-2.856938
35	6	0	-4.460426	2.958318	-1.091504
36	6	0	-3.642701	2.722401	-2.250798
37	6	0	-2.522761	2.501789	0.377142
38	6	0	-2.314180	-0.271591	2.386502
39	6	0	-0.470299	-1.366258	1.124814
40	6	0	-4.458784	2.181446	-3.297124
41	6	0	-3.985480	1.064547	-3.995423
42	6	0	-2.686313	0.491590	-3.703300
43	6	0	-4.904257	0.014606	-4.359309
44	6	0	-5.297498	-3.885422	-2.137591
45	6	0	-0.415148	1.681675	-0.974885
46	6	0	-6.314541	-2.310990	-3.550275
47	6	0	-4.907607	-2.392042	-3.903733
48	6	0	-1.732967	2.324035	-0.763996
49	6	0	-1.523344	-2.281669	0.607012
50	6	0	-1.594364	-2.637669	-0.743728
51	6	0	-2.355811	2.256133	-2.069710
52	6	0	-1.826853	1.185838	-2.872224
53	6	0	-4.198046	-1.244038	-4.259758
54	6	0	-2.836521	-0.994618	-3.793053
55	6	0	-0.608788	0.659219	-2.153376

56	6	0	-4.287074	-3.356751	-3.041673	111	1	0	-1.799970	8.342913	3.767662
57	6	0	-2.643392	-3.461999	-1.219834	112	1	0	-3.519362	8.358979	3.316986
58	6	0	-1.086088	-1.787732	-1.946195	113	1	0	-3.112403	7.983884	0.258137
59	6	0	-2.996601	-3.108828	-2.582609	114	1	0	-4.313737	7.108374	1.226146
60	6	0	-2.239843	-1.949852	-2.974709	115	1	0	-3.151979	6.206737	0.233585
61	6	0	-2.091638	2.212443	1.841593	116	1	0	-0.670411	7.975217	0.896085
62	6	0	-0.815651	-0.498777	2.379414	117	1	0	-0.649985	6.198390	0.869182
63	6	0	-0.057514	0.804307	2.339836	118	1	0	-0.100314	7.071664	2.311199
64	6	0	-0.613540	1.983007	2.059883	119	6	0	3.116137	2.789461	-3.268362
65	6	0	-0.380499	-1.321569	3.614318	120	6	0	3.422803	3.202391	-1.979897
66	6	0	-2.448633	3.436948	2.718843	121	6	0	4.137973	2.354889	-1.131234
67	8	0	0.623279	-1.259729	0.576391	122	6	0	4.557913	1.069765	-1.489731
68	8	0	0.656144	1.781136	-0.403229	123	6	0	4.240611	0.720747	-2.809174
69	7	0	-2.287186	4.622819	2.130649	124	6	0	3.533024	1.530829	-3.688535
70	6	0	-2.490581	5.754605	2.830702	125	6	0	8.747705	-0.456596	-2.932215
71	6	0	-2.868936	5.704177	4.178690	126	6	0	7.569729	-0.693097	-2.222674
72	6	0	-3.028800	4.463407	4.794716	127	6	0	6.989941	0.234848	-1.356031
73	6	0	-2.813473	3.300646	4.061410	128	6	0	7.671496	1.454010	-1.283706
74	6	0	-0.342076	-0.744836	4.886387	129	6	0	8.847230	1.735493	-1.969752
75	6	0	0.084878	-1.544052	5.941642	130	6	0	9.393963	0.766148	-2.805442
76	6	0	0.457893	-2.866374	5.697754	131	6	0	5.005873	-1.510335	-0.504020
77	6	0	0.390761	-3.370013	4.392870	132	6	0	5.836883	-2.489559	0.061411
78	7	0	-0.032658	-2.588052	3.380652	133	6	0	5.450281	-3.803112	0.310897
79	8	0	-0.983905	-0.486929	-1.392677	134	6	0	4.152256	-4.208734	0.008814
80	8	0	0.584299	0.508601	-2.837617	135	6	0	3.283458	-3.279819	-0.541132
81	8	0	0.106698	-2.204617	-2.554753	136	6	0	3.732079	-1.985467	-0.779564
82	6	0	-2.279407	7.058572	2.049209	137	6	0	4.292232	0.837315	3.114431
83	6	0	0.770030	-4.806809	4.008032	138	6	0	5.462442	0.931121	3.859189
84	6	0	1.809981	-4.765318	2.865069	139	6	0	6.679665	0.782472	3.206095
85	6	0	-0.504058	-5.531373	3.513886	140	6	0	6.712753	0.545200	1.829693
86	6	0	1.361829	-5.589077	5.194175	141	6	0	5.568835	0.463181	1.026984
87	6	0	-2.497575	8.306417	2.922649	142	6	0	4.389310	0.600388	1.751955
88	6	0	-3.277210	7.088233	0.868293	143	5	0	5.536733	0.070603	-0.591760
89	6	0	-0.835157	7.073646	1.497428	144	9	0	3.167510	0.507106	1.102474
90	3	0	1.813044	0.168397	-0.244236	145	9	0	3.094345	0.968846	3.717057
91	1	0	1.008509	0.748749	2.531438	146	9	0	5.411400	1.154011	5.178507
92	1	0	0.009269	2.870662	2.008553	147	9	0	7.818522	0.855911	3.907124
93	1	0	-3.033888	6.613324	4.743916	148	9	0	7.941440	0.388378	1.310902
94	1	0	-3.318546	4.406064	5.840648	149	9	0	7.093757	-2.169000	0.415423
95	1	0	-2.928440	2.320941	4.513078	150	9	0	6.305416	-4.677666	0.855055
96	1	0	-0.620382	0.293332	5.035676	151	9	0	3.743983	-5.457596	0.267507
97	1	0	0.136714	-1.139814	6.949015	152	9	0	2.006087	-3.633208	-0.823579
98	1	0	0.801523	-3.488926	6.514677	153	9	0	2.760059	-1.152912	-1.320378
99	1	0	0.617979	-0.393571	-3.213882	154	9	0	7.180603	2.445173	-0.505052
100	1	0	0.761795	-2.416957	-1.861133	155	9	0	9.451625	2.927543	-1.841788
101	1	0	2.076192	-5.782286	2.557077	156	9	0	10.525099	1.012069	-3.480986
102	1	0	2.728898	-4.261006	3.187363	157	9	0	9.254976	-1.399522	-3.742637
103	1	0	1.418009	-4.234869	1.993462	158	9	0	7.003757	-1.902285	-2.432184
104	1	0	-0.257147	-6.549714	3.191602	159	9	0	4.606597	-0.491898	-3.282524
105	1	0	-0.952432	-5.001420	2.668679	160	9	0	3.223653	1.099822	-4.921548
106	1	0	-1.254722	-5.600926	4.310370	161	9	0	2.405622	3.578215	-4.085501
107	1	0	1.636615	-6.597568	4.867062	162	9	0	3.013549	4.406468	-1.549339
108	1	0	0.644499	-5.697037	6.016301	163	9	0	4.387177	2.857485	0.097878
109	1	0	2.267687	-5.112527	5.586679	----------					
110	1	0	-2.332205	9.207655	2.322406	The total electronic energy was calculated to be –6570.6800899 Hartree.					

11. Optimized Structures of $Li^+\subset(1)_2$

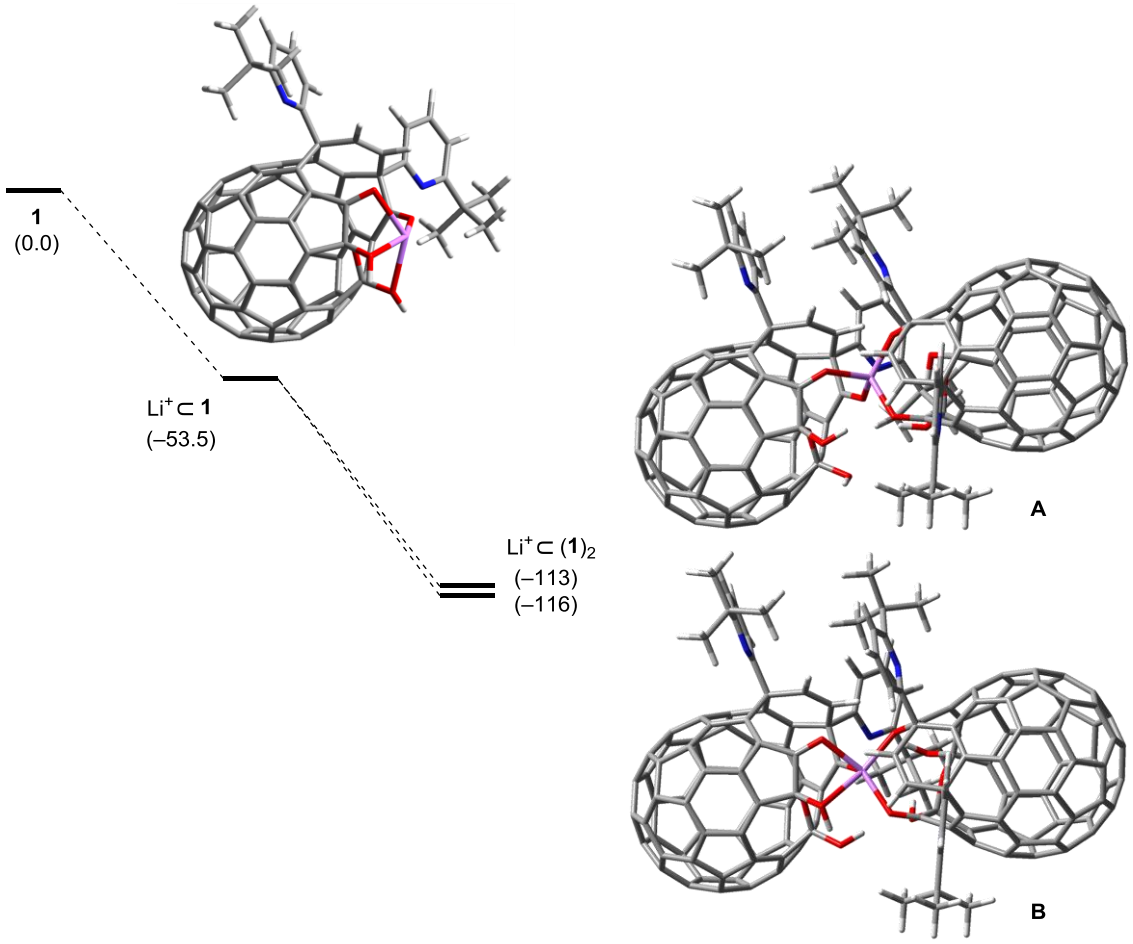
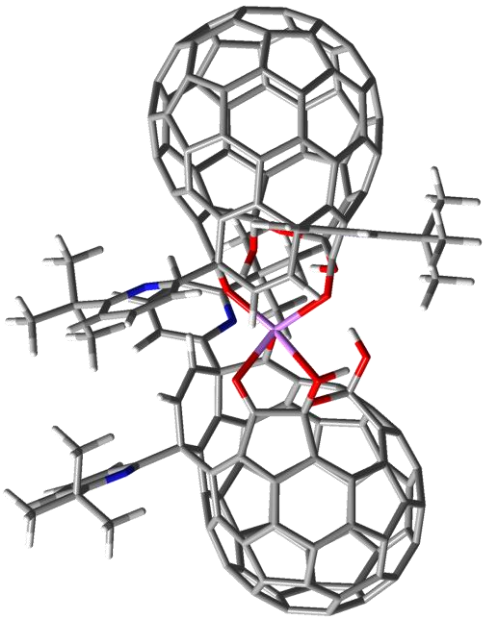


Figure S15. Optimized structures of $Li^+\subset(\mathbf{1})_2$ calculated at the M06-2X/6-31G(d,p) level of theory. The values in parentheses are differences in Gibbs energies at 298 K (units in kcal/mol).

Table S22. Optimized structure of $Li^{+}\subset(\mathbf{1A})_2$ (M06-2X/6-31G(d,p))



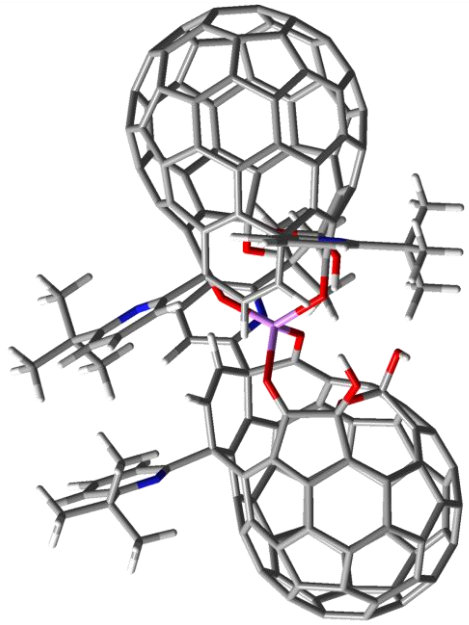
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	9.567164	-0.263450	0.077316
2	6	0	8.810010	0.285193	1.186940
3	6	0	8.235707	1.531165	1.067935
4	6	0	8.359137	2.286102	-0.163244
5	6	0	9.043046	1.746523	-1.241240
6	6	0	9.663874	0.441090	-1.116409
7	6	0	8.078136	-0.786423	1.834881
8	6	0	6.925796	1.751567	1.616535
9	6	0	7.105389	2.972302	-0.364455
10	6	0	8.481460	1.855723	-2.574016
11	6	0	9.495430	-0.254539	-2.378045
12	6	0	9.349823	-1.691730	0.064810
13	6	0	7.268523	2.508659	-2.761669
14	6	0	6.567537	3.083875	-1.631529
15	6	0	6.273235	1.940202	-3.644277
16	6	0	5.144963	2.880985	-1.808800
17	6	0	6.782475	-0.600546	2.340030
18	6	0	6.230608	2.673984	0.745962
19	6	0	4.974481	2.169212	-3.047214
20	6	0	4.854783	2.590071	0.612428
21	6	0	6.216854	0.743508	2.263792
22	6	0	8.750580	0.613503	-3.271990
23	6	0	9.269292	-1.624504	-2.390962
24	6	0	5.831386	-1.723822	2.282450
25	6	0	9.215777	-2.366107	-1.145045
26	6	0	8.471633	-2.013899	1.169603
27	6	0	8.276194	-2.187800	-3.285084
28	6	0	8.223115	-3.409970	-1.281589
29	6	0	7.563571	-3.041704	1.053876
30	6	0	4.281031	2.649379	-0.734241
31	6	0	7.792473	0.071473	-4.123237
32	6	0	4.789186	0.915999	2.387695
33	6	0	7.618097	-3.280017	-2.596532
34	6	0	7.438924	-3.766796	-0.197692
35	6	0	6.251821	-2.890606	1.632887
36	6	0	5.339160	-3.612044	0.788258
37	6	0	4.400006	-1.462072	2.406606
38	6	0	4.136474	1.847094	1.622092
39	6	0	2.158983	1.624159	0.162725
40	6	0	6.035736	-4.058607	-0.378412
41	6	0	5.438654	-3.861043	-1.620854
42	6	0	4.129175	-3.260236	-1.736777
43	6	0	6.249706	-3.463341	-2.742416
44	6	0	6.523592	0.743997	-4.297901
45	6	0	2.150446	-1.941576	1.126576
46	6	0	7.542750	-1.358599	-4.118059
47	6	0	6.112922	-1.561679	-4.265299
48	6	0	3.524059	-2.205077	1.628766
49	6	0	3.104293	1.832927	-0.957965
50	6	0	3.052367	1.025442	-2.083076
51	6	0	4.043644	-3.166086	0.681312
52	6	0	3.391685	-3.073220	-0.594132
53	6	0	5.463924	-2.564444	-3.558143
54	6	0	4.162133	-2.359586	-2.933386
55	6	0	2.199134	-2.174686	-0.415412
56	6	0	5.490454	-0.276854	-4.378132
57	6	0	3.992592	1.191059	-3.126340
58	6	0	2.508405	-0.427653	-2.152684
59	6	0	4.261545	-0.078134	-3.771371
60	6	0	3.558340	-1.118856	-3.066711
61	6	0	4.053040	-0.165632	3.162852
62	6	0	2.630304	1.981159	1.588235
63	6	0	1.954892	1.094577	2.599522
64	6	0	2.578828	0.128430	3.266194
65	6	0	2.238407	3.448703	1.826504
66	6	0	4.564693	-0.291729	4.607542
67	8	0	1.044266	1.166012	-0.037589
68	8	0	1.120553	-1.591597	1.659073
69	7	0	4.457023	-1.506588	5.132179
70	6	0	4.830560	-1.714561	6.402940
71	6	0	5.316606	-0.667379	7.190357
72	6	0	5.409013	0.607222	6.640442
73	6	0	5.027099	0.812288	5.320927
74	6	0	2.335939	4.002814	3.101841
75	6	0	1.985975	5.337459	3.244917
76	6	0	1.564075	6.059519	2.130617
77	6	0	1.501241	5.423965	0.889667
78	7	0	1.834963	4.129771	0.760750
79	8	0	2.533948	-0.862136	-0.813273
80	8	0	0.973512	-2.634522	-0.860139
81	8	0	1.237245	-0.565602	-2.702361
82	6	0	4.690573	-3.153790	6.889781
83	6	0	1.056533	6.109790	-0.399327
84	6	0	-0.236676	5.431698	-0.880727
85	6	0	2.154678	5.918056	-1.457749
86	6	0	0.802058	7.604900	-0.197533
87	6	0	5.138457	-3.317954	8.343439
88	6	0	5.552124	-4.049416	5.984409
89	6	0	3.216106	-3.567704	6.759321
90	1	0	0.892198	1.267155	2.761001
91	1	0	2.023113	-0.505029	3.952266

92	1	0	5.619185	-0.840659	8.215344	164	6	0	-6.281904	-4.557794	1.782877
93	1	0	5.781984	1.433270	7.237611	165	6	0	-3.832509	1.439806	1.883444
94	1	0	5.094508	1.789250	4.853712	166	6	0	-2.960161	-1.674788	-1.687462
95	1	0	2.669735	3.399619	3.940113	167	6	0	-2.976985	-2.692988	-0.749498
96	1	0	2.041588	5.818019	4.216434	168	6	0	-4.432267	0.608938	2.902391
97	1	0	1.292777	7.102832	2.231470	169	6	0	-3.756504	-0.653931	3.048614
98	1	0	0.762577	-2.218251	-1.714117	170	6	0	-5.746023	-3.706629	2.739520
99	1	0	0.625343	-0.026567	-2.166579	171	6	0	-4.435320	-3.086624	2.583955
100	1	0	-0.549810	5.855217	-1.840689	172	6	0	-2.493875	-0.563429	2.232931
101	1	0	-1.050073	5.581631	-0.161729	173	6	0	-5.527831	-4.831194	0.596454
102	1	0	-0.075356	4.357137	-1.007699	174	6	0	-3.889689	-3.765461	-0.867537
103	1	0	1.851882	6.388994	-2.398007	175	6	0	-2.592727	-2.546264	0.742439
104	1	0	2.334285	4.855208	-1.637804	176	6	0	-4.288045	-4.234106	0.444173
105	1	0	3.095024	6.374890	-1.133485	177	6	0	-3.705689	-3.374483	1.442573
106	1	0	0.500369	8.055117	-1.147253	178	6	0	-4.148369	2.670959	-0.384958
107	1	0	1.702172	8.124042	0.146740	179	6	0	-2.488527	0.840618	-2.116278
108	1	0	-0.000910	7.785118	0.524307	180	6	0	-1.918885	1.948673	-1.276238
109	1	0	5.021376	-4.362456	8.644812	181	6	0	-2.650945	2.737819	-0.500645
110	1	0	4.536517	-2.706907	9.023741	182	6	0	-1.900230	0.891582	-3.537205
111	1	0	6.192008	-3.051253	8.474730	183	6	0	-4.642647	4.122670	-0.495418
112	1	0	5.439382	-5.097322	6.278810	184	8	0	-0.974944	-0.623930	-0.953446
113	1	0	6.610820	-3.783182	6.065058	185	8	0	-1.367316	1.455014	1.577075
114	1	0	5.247625	-3.941183	4.940298	186	7	0	-4.402695	4.851115	0.591323
115	1	0	3.093391	-4.611870	7.062787	187	6	0	-4.732927	6.148355	0.607316
116	1	0	2.880922	-3.460342	5.725024	188	6	0	-5.323387	6.755127	-0.505556
117	1	0	2.577986	-2.948699	7.398021	189	6	0	-5.555532	5.993433	-1.645076
118	6	0	-9.615467	-0.503717	-0.440341	190	6	0	-5.208098	4.647349	-1.654609
119	6	0	-8.814122	0.539247	-1.053068	191	6	0	-1.710056	2.106644	-4.190543
120	6	0	-8.108753	0.267163	-2.203954	192	6	0	-1.164476	2.062274	-5.467043
121	6	0	-8.141100	-1.056343	-2.793403	193	6	0	-0.843124	0.833241	-6.035794
122	6	0	-8.870838	-2.067490	-2.187741	194	6	0	-1.080599	-0.338596	-5.312875
123	6	0	-9.626957	-1.782969	-0.982566	195	7	0	-1.597389	-0.285798	-4.076570
124	6	0	-8.206397	1.342720	-0.009555	196	8	0	-2.705508	-1.151288	0.966955
125	6	0	-6.786925	0.810937	-2.359152	197	8	0	-1.266135	-0.884176	2.782231
126	6	0	-6.819688	-1.319584	-3.310188	198	8	0	-1.344035	-3.036296	1.102353
127	6	0	-8.291264	-3.390332	-2.057086	199	6	0	-4.404242	6.883226	1.904425
128	6	0	-9.523052	-2.936276	-0.108883	200	6	0	-0.846278	-1.741407	-5.866635
129	6	0	-9.549312	-0.320238	0.991240	201	6	0	-0.066517	-2.579317	-4.842465
130	6	0	-7.014679	-3.637173	-2.549181	202	6	0	-2.227917	-2.380368	-6.092412
131	6	0	-6.264586	-2.578267	-3.193701	203	6	0	-0.076311	-1.714909	-7.189276
132	6	0	-6.079084	-4.416692	-1.768446	204	6	0	-4.865821	8.341660	1.875249
133	6	0	-4.870505	-2.696811	-2.820902	205	6	0	-5.093893	6.151517	3.066734
134	6	0	-6.904545	1.851039	-0.127660	206	6	0	-2.879830	6.835582	2.103739
135	6	0	-5.989741	-0.160333	-3.074209	207	1	0	-0.836460	2.050258	-1.282029
136	6	0	-4.767173	-3.830331	-1.940893	208	1	0	-2.172201	3.485790	0.124043
137	6	0	-4.629274	-0.250477	-2.828423	209	1	0	-5.595307	7.802947	-0.486443
138	6	0	-6.194964	1.606298	-1.381865	210	1	0	-6.006856	6.447059	-2.521806
139	6	0	-8.684237	-3.921913	-0.766354	211	1	0	-5.376007	4.026471	-2.527340
140	6	0	-9.441738	-2.760692	1.266081	212	1	0	-1.974805	3.041207	-3.706727
141	6	0	-6.079880	1.969845	1.086730	213	1	0	-0.989867	2.979970	-6.019663
142	6	0	-9.476701	-1.425796	1.833282	214	1	0	-0.415480	0.791244	-7.029537
143	6	0	-8.720193	0.837944	1.250005	215	1	0	-1.090097	-1.835868	2.677905
144	6	0	-8.506005	-3.549263	2.044653	216	1	0	-0.672508	-2.765332	0.443326
145	6	0	-8.596918	-1.399343	2.981768	217	1	0	0.037719	-3.604571	-5.210180
146	6	0	-7.924454	0.880915	2.372559	218	1	0	0.930652	-2.163886	-4.671812
147	6	0	-4.045646	-1.581805	-2.642359	219	1	0	-0.599426	-2.602296	-3.887152
148	6	0	-7.782296	-4.672490	-0.018391	220	1	0	-2.110934	-3.397369	-6.479372
149	6	0	-4.757968	1.742800	-1.422616	221	1	0	-2.786089	-2.426237	-5.152810
150	6	0	-7.970234	-2.705557	3.093785	222	1	0	-2.814011	-1.803781	-6.814878
151	6	0	-7.864430	-0.260051	3.267962	223	1	0	0.103752	-2.739378	-7.526123
152	6	0	-6.610490	1.466483	2.280902	224	1	0	-0.638775	-1.205579	-7.977882
153	6	0	-5.768474	0.744335	3.195889	225	1	0	0.895079	-1.222144	-7.078778
154	6	0	-4.633067	2.091112	0.958211	226	1	0	-4.622117	8.820733	2.827496
155	6	0	-4.001154	0.867373	-2.162566	227	1	0	-4.368451	8.909115	1.082088
156	6	0	-2.051600	-0.517646	-1.529278	228	1	0	-5.948251	8.418686	1.732042
157	6	0	-6.497019	-0.368648	3.721115	229	1	0	-4.832866	6.628404	4.016451
158	6	0	-5.870479	-1.611427	3.754443	230	1	0	-6.182258	6.183970	2.955807
159	6	0	-4.504151	-1.776958	3.308279	231	1	0	-4.781797	5.105021	3.097791
160	6	0	-6.626794	-2.794246	3.433192	232	1	0	-2.607944	7.323421	3.045211
161	6	0	-6.448852	-4.909906	-0.526908	233	1	0	-2.528778	5.800225	2.130583
162	6	0	-2.433682	0.945379	1.834374	234	1	0	-2.368300	7.357134	1.287180
163	6	0	-7.683500	-4.469708	1.415894	235	3	0	-0.117446	-0.077159	0.915706

The total electronic energy was calculated to be –7259.1300224 Hartree.

Table S23. Optimized structure of $Li^{+}\subset(\mathbf{1B})_2$ (M06-2X/6-31G(d,p))



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	9.556612	-0.323869	0.515083
2	6	0	8.777961	0.694630	1.194996
3	6	0	8.279044	1.759538	0.478688
4	6	0	8.498916	1.855226	-0.951270
5	6	0	9.200305	0.859449	-1.612610
6	6	0	9.744964	-0.254921	-0.859874
7	6	0	7.959207	0.062786	2.212328
8	6	0	6.960067	2.244387	0.778427
9	6	0	7.294194	2.402706	-1.526726
10	6	0	8.705011	0.352645	-2.878054
11	6	0	9.598797	-1.451180	-1.667321
12	6	0	9.266199	-1.589800	1.147687
13	6	0	7.536087	0.873454	-3.421344
14	6	0	6.817395	1.925031	-2.731829
15	6	0	6.551815	-0.014854	-4.000870
16	6	0	5.395169	1.696707	-2.883148
17	6	0	6.651779	0.492775	2.486084
18	6	0	6.357176	2.678651	-0.462950
19	6	0	5.241801	0.494906	-3.657078
20	6	0	4.986875	2.578979	-0.630224
21	6	0	6.168081	1.666748	1.767813
22	6	0	8.940614	-1.077850	-2.906174
23	6	0	9.304018	-2.665654	-1.062399
24	6	0	5.642226	-0.506081	2.883843
25	6	0	9.153970	-2.744132	0.378879
26	6	0	8.320110	-1.341797	2.214991
27	6	0	8.327275	-3.555625	-1.659194
28	6	0	8.117216	-3.709035	0.674852
29	6	0	7.367037	-2.283543	2.528031
30	6	0	4.474323	2.011199	-1.880945
31	6	0	7.994632	-1.928359	-3.470243
32	6	0	4.749191	1.918480	1.708450
33	6	0	7.584180	-4.189821	-0.589253
34	6	0	7.265674	-3.503691	1.747940
35	6	0	6.037469	-1.849193	2.880401
36	6	0	5.131634	-2.859484	2.409433
37	6	0	4.219674	-0.181836	2.773984
38	6	0	4.188231	2.417648	0.561834
39	6	0	2.272708	1.599633	-0.752262
40	6	0	5.860178	-3.814247	1.630950
41	6	0	5.338539	-4.205300	0.400179
42	6	0	4.071742	-3.697834	-0.066909
43	6	0	6.217505	-4.390071	-0.724177
44	6	0	6.769151	-1.382806	-4.012978
45	6	0	1.998023	-1.180780	1.710464
46	6	0	7.674065	-3.188096	-2.825031
47	6	0	6.243886	-3.402551	-2.954415
48	6	0	3.336871	-1.180446	2.372301
49	6	0	3.267121	1.212562	-1.775014
50	6	0	3.215479	-0.024318	-2.402244
51	6	0	3.869660	-2.480246	2.019021
52	6	0	3.303410	-2.976062	0.804823
53	6	0	5.513979	-3.950450	-1.910178
54	6	0	4.195323	-3.450852	-1.535975
55	6	0	2.126541	-2.125749	0.470138
56	6	0	5.689588	-2.298733	-3.679458
57	6	0	4.214055	-0.383077	-3.337991
58	6	0	2.565901	-1.329341	-1.860857
59	6	0	4.444997	-1.813120	-3.309820
60	6	0	3.653295	-2.393638	-2.253365
61	6	0	3.915070	1.326511	2.835108
62	6	0	2.701512	2.565169	0.369087
63	6	0	1.925138	2.253767	1.620945
64	6	0	2.456905	1.672936	2.691142
65	6	0	2.351191	3.981796	-0.116479
66	6	0	4.342515	1.848872	4.216987
67	8	0	1.134201	1.168395	-0.779178
68	8	0	0.942017	-0.609075	1.923832
69	7	0	4.077336	1.023612	5.223508
70	6	0	4.363160	1.396250	6.478902
71	6	0	4.921889	2.648746	6.747804
72	6	0	5.179752	3.515920	5.691122
73	6	0	4.887531	3.118834	4.392356
74	6	0	2.529193	5.077693	0.726981
75	6	0	2.163564	6.323335	0.238688
76	6	0	1.642484	6.430334	-1.049712
77	6	0	1.502122	5.279515	-1.826645
78	7	0	1.862213	4.077916	-1.346776
79	8	0	2.456498	-1.115828	-0.470859
80	8	0	1.031601	-2.881523	0.150235
81	8	0	1.335208	-1.532876	-2.460437
82	6	0	4.043482	0.357332	7.549912
83	6	0	0.950788	5.267144	-3.250575
84	6	0	-0.276536	4.341326	-3.290551
85	6	0	2.040309	4.704888	-4.178781
86	6	0	0.548196	6.663756	-3.728802
87	6	0	4.394708	0.849484	8.955303
88	6	0	4.849453	-0.914007	7.236325
89	6	0	2.541844	0.036964	7.481374
90	1	0	0.868364	2.501661	1.598202
91	1	0	1.837741	1.437018	3.553085
92	1	0	5.153188	2.944774	7.763203
93	1	0	5.611169	4.493659	5.880742
94	1	0	5.085115	3.763655	3.542654

95	1	0	2.929739	4.943261	1.726909	167	6	0	-3.331060	-2.919454	0.547223
96	1	0	2.278790	7.209563	0.854494	168	6	0	-4.373422	1.738000	2.391172
97	1	0	1.348777	7.398118	-1.437385	169	6	0	-3.895000	0.588782	3.105540
98	1	0	0.195622	-2.413093	0.336611	170	6	0	-6.281455	-2.043236	3.934308
99	1	0	0.925994	-2.332083	-2.089748	171	6	0	-4.893677	-1.708084	3.636734
100	1	0	-0.672757	4.286344	-4.309983	172	6	0	-2.611928	0.168032	2.457078
101	1	0	-1.076104	4.714656	-2.638373	173	6	0	-6.179964	-3.978297	2.469303
102	1	0	-0.001781	3.333709	-2.966029	174	6	0	-4.384070	-3.824842	0.818558
103	1	0	1.662762	4.642844	-5.204086	175	6	0	-2.944421	-2.218373	1.874487
104	1	0	2.341185	3.705563	-3.853628	176	6	0	-4.867247	-3.649237	2.173596
105	1	0	2.925120	5.349087	-4.178240	177	6	0	-4.187626	-2.527662	2.769474
106	1	0	0.171846	6.601821	-4.753701	178	6	0	-3.721434	2.133863	-1.425078
107	1	0	1.397584	7.354064	-3.728593	179	6	0	-2.349445	-0.435989	-2.198944
108	1	0	-0.248751	7.091073	-3.110066	180	6	0	-1.621934	0.848575	-1.934092
109	1	0	4.148947	0.073275	9.685108	181	6	0	-2.224536	1.951001	-1.500543
110	1	0	3.828730	1.747626	9.222732	182	6	0	-1.782560	-1.123034	-3.450220
111	1	0	5.462803	1.068716	9.051837	183	6	0	-3.954432	3.465254	-2.158977
112	1	0	4.608529	-1.697878	7.960887	184	8	0	-1.074065	-1.320904	-0.379045
113	1	0	5.924963	-0.717685	7.289355	185	8	0	-1.195660	1.533079	1.061212
114	1	0	4.614180	-1.276358	6.232325	186	7	0	-3.715818	4.538901	-1.413282
115	1	0	2.291487	-0.737384	8.212915	187	6	0	-3.754252	5.756640	-1.969840
116	1	0	2.274806	-0.321603	6.484459	188	6	0	-4.036019	5.916898	-3.329880
117	1	0	1.941430	0.924716	7.704166	189	6	0	-4.286193	4.788877	-4.105255
118	6	0	-9.601615	-0.045764	-0.576961	190	6	0	-4.244615	3.529067	-3.519581
119	6	0	-8.650133	0.533831	-1.506850	191	6	0	-1.649064	-0.414292	-4.641455
120	6	0	-7.976432	-0.282568	-2.387345	192	6	0	-1.122509	-1.094199	-5.730008
121	6	0	-8.188708	-1.717222	-2.372613	193	6	0	-0.765945	-2.434026	-5.596357
122	6	0	-9.059682	-2.279916	-1.453258	194	6	0	-0.942033	-3.068242	-4.365882
123	6	0	-9.786133	-1.422374	-0.535862	195	7	0	-1.439511	-2.399420	-3.313283
124	6	0	-7.947788	1.619656	-0.849610	196	8	0	-2.851348	-0.858583	1.515918
125	6	0	-6.589795	-0.020627	-2.659835	197	8	0	-1.592855	-0.097044	3.341227
126	6	0	-6.911597	-2.334105	-2.636248	198	8	0	-1.756686	-2.726665	2.375007
127	6	0	-8.671217	-3.481452	-0.740090	199	6	0	-3.472843	6.910205	-1.010995
128	6	0	-9.859946	-2.101262	0.743857	200	6	0	-0.629108	-4.540950	-4.111090
129	6	0	-9.533310	0.716091	0.648242	201	6	0	0.356840	-4.652612	-2.937607
130	6	0	-7.433032	-4.063679	-0.987923	202	6	0	-1.943185	-5.244039	-3.730974
131	6	0	-6.533824	-3.477910	-1.960759	203	6	0	-0.025644	-5.220650	-5.342042
132	6	0	-6.626715	-4.540759	0.114426	204	6	0	-3.462910	8.263777	-1.723655
133	6	0	-5.174446	-3.590629	-1.471019	205	6	0	-4.566908	6.905718	0.069571
134	6	0	-6.583196	1.863194	-1.069446	206	6	0	-2.106054	6.670681	-0.349402
135	6	0	-5.933001	-1.295240	-2.849855	207	1	0	-0.545599	0.821794	-2.067884
136	6	0	-5.244218	-4.239389	-0.189213	208	1	0	-1.634031	2.827229	-1.246607
137	6	0	-4.603863	-1.439445	-2.494628	209	1	0	-4.060936	6.902111	-3.778474
138	6	0	-5.902222	1.032595	-2.058269	210	1	0	-4.509349	4.893080	-5.162382
139	6	0	-9.156016	-3.365069	0.621684	211	1	0	-4.428148	2.627348	-4.094017
140	6	0	-9.778518	-1.371852	1.922397	212	1	0	-1.939939	0.630225	-4.696077
141	6	0	-5.765022	2.375457	0.044682	213	1	0	-0.990529	-0.588412	-6.681161
142	6	0	-9.633726	0.071124	1.877224	214	1	0	-0.357593	-2.972976	-6.441780
143	6	0	-8.549955	1.762356	0.462229	215	1	0	-0.740330	-0.067109	2.870140
144	6	0	-8.978243	-1.863723	3.027106	216	1	0	-1.601692	-2.319036	3.239912
145	6	0	-8.780956	0.475013	2.974019	217	1	0	0.563893	-5.704636	-2.720153
146	6	0	-7.775982	2.179729	1.520579	218	1	0	1.309614	-4.166657	-3.177769
147	6	0	-4.203501	-2.616799	-1.718280	219	1	0	-0.063977	-4.202417	-2.032152
148	6	0	-8.380480	-3.830081	1.679203	220	1	0	-1.754421	-6.300942	-3.519389
149	6	0	-4.460961	0.958553	-2.048835	221	1	0	-2.382272	-4.781553	-2.842736
150	6	0	-8.349524	-0.726686	3.668344	222	1	0	-2.670017	-5.181888	-4.546867
151	6	0	-7.898949	1.530422	2.813622	223	1	0	0.188243	-6.267906	-5.112180
152	6	0	-6.388534	2.501624	1.293920	224	1	0	-0.715277	-5.203146	-6.191653
153	6	0	-5.680841	2.146977	2.493448	225	1	0	0.913556	-4.746755	-5.645035
154	6	0	-4.311368	2.245439	-0.007369	226	1	0	-3.246683	9.055709	-1.001345
155	6	0	-3.836808	-0.231902	-2.325045	227	1	0	-2.694483	8.304115	-2.503234
156	6	0	-2.107989	-1.410653	-1.032090	228	1	0	-4.432018	8.488569	-2.179994
157	6	0	-6.571652	1.460728	3.377984	229	1	0	-4.370771	7.691642	0.805401
158	6	0	-6.131929	0.282976	3.976846	230	1	0	-5.551931	7.087737	-0.371335
159	6	0	-4.795630	-0.219147	3.750328	231	1	0	-4.590899	5.940293	0.581570
160	6	0	-7.039905	-0.825230	4.118137	232	1	0	-1.898242	7.461023	0.378945
161	6	0	-7.083229	-4.414600	1.416644	233	1	0	-2.090710	5.705243	0.162410
162	6	0	-2.325677	1.325097	1.452529	234	1	0	-1.302074	6.674894	-1.093819
163	6	0	-8.280679	-3.054595	2.902148	235	3	0	-0.025578	0.173947	0.280377
164	6	0	-6.911953	-3.146416	3.377092						
165	6	0	-3.633807	1.964979	1.170859						
166	6	0	-3.150015	-2.417397	-0.734217						

The total electronic energy was calculated to be –7259.1275622 Hartree

12. References

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