Supporting Information

Crystallographic Structure Determination of Both [5,6]- and [6,6]-Isomers of Lithium-ion-containing Dipheylmethano[60]fullerene

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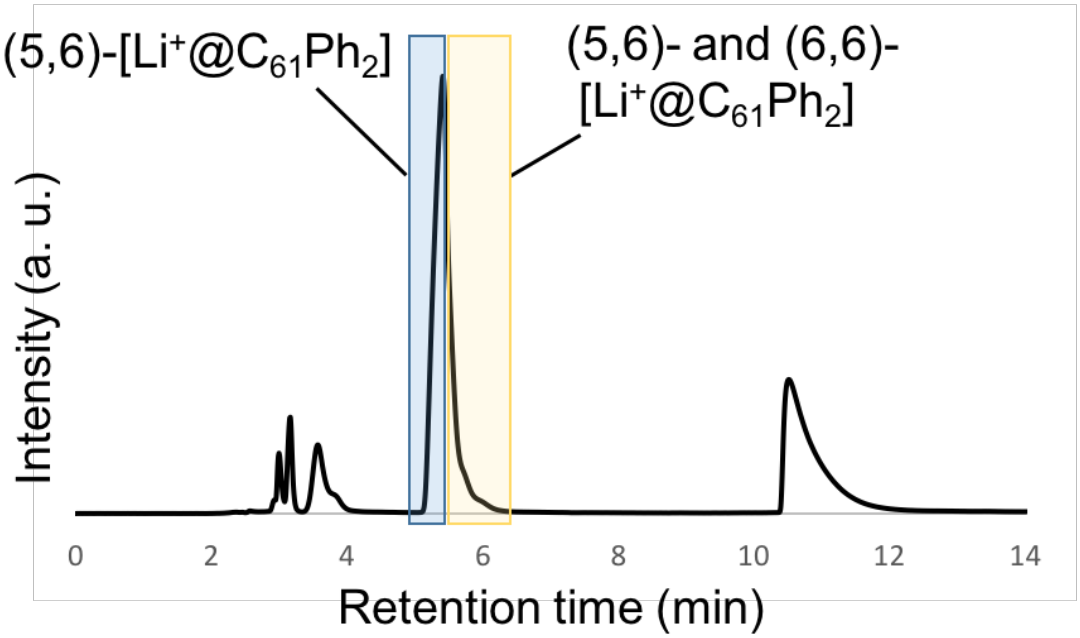


Figure S1. Preparative HPLC chart for separation of [5,6]- and [6,6]-$[Li^+@C_{61}Ph_2]TFSI^-$. Column: Inertsil CX, φ10 × 250 mm, GL Science; flow rate: 7.0 mL/min; eluent: (A) chlorobenzene:acetonitrile = 1:1 v/v containing 10 mM LiTFSI, (B) acetonitrile containing 10 mM LiTFSI; gradient: A/B = 35/65 to 70/30 (5–10 min), A/B=70/30 (after 10 min).

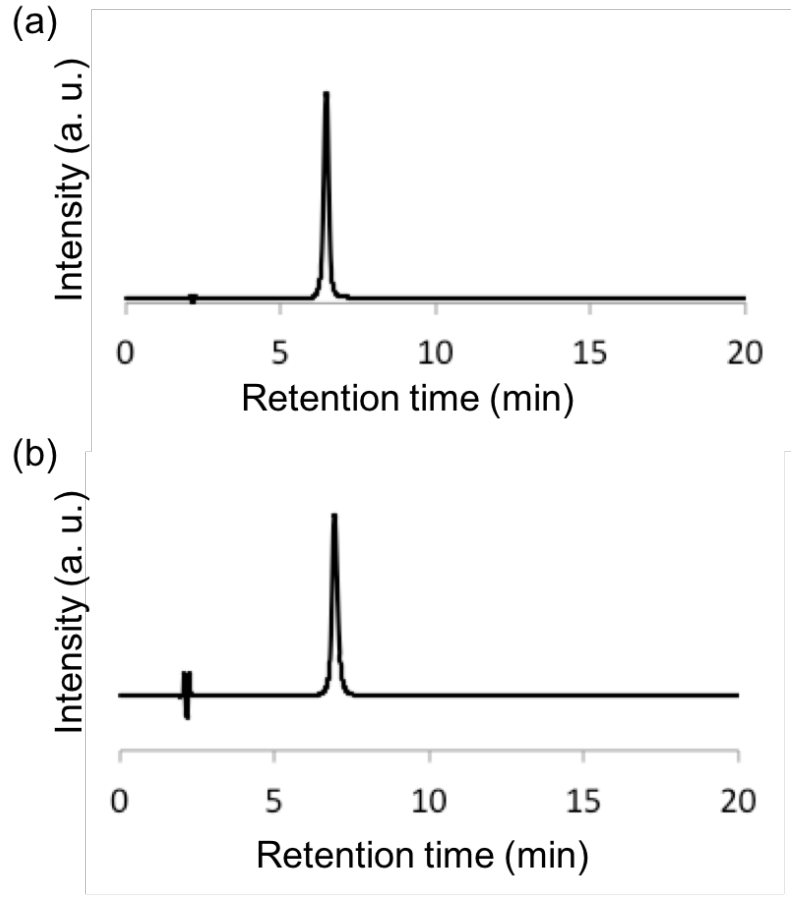


Figure S2. Analytical HPLC charts of pure (a) [5,6]- and (b) [6,6]-[Li^{+}@$C_{61}Ph_2$]$TFSI^{-}$. Column: Inertsil CX, φ4.6 × 250 mm, GL Science; flow rate: 1.5 mL/min; eluent: chlorobenzene:acetonitrile = 1:3 v/v containing 2.5 mM LiTFSI.

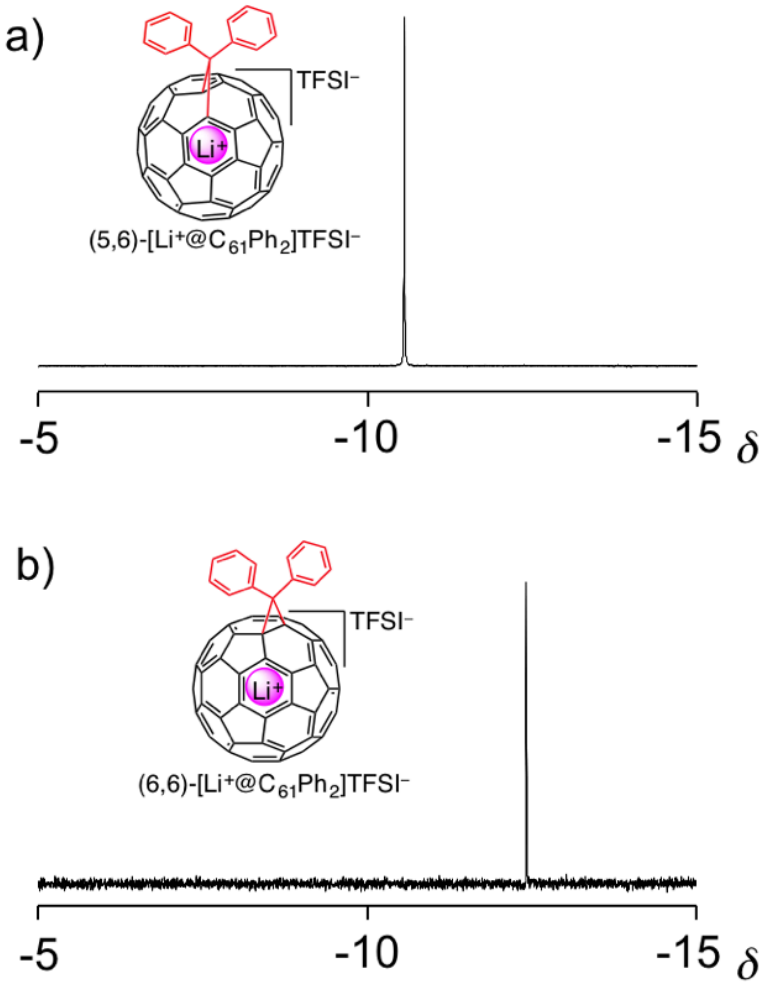


Figure S3. The ^{7}Li NMR (115 MHz) spectra of [5,6]- and [6,6]-[Li^{+}@$C_{61}Ph_2$]$TFSI^{-}$ in 1,2-dichlorobenzene-d_4. (a) [5,6]-[Li^{+}@$C_{61}Ph_2$]$TFSI^{-}$. (b) [6,6]-[Li^{+}@$C_{61}Ph_2$]$TFSI^{-}$.

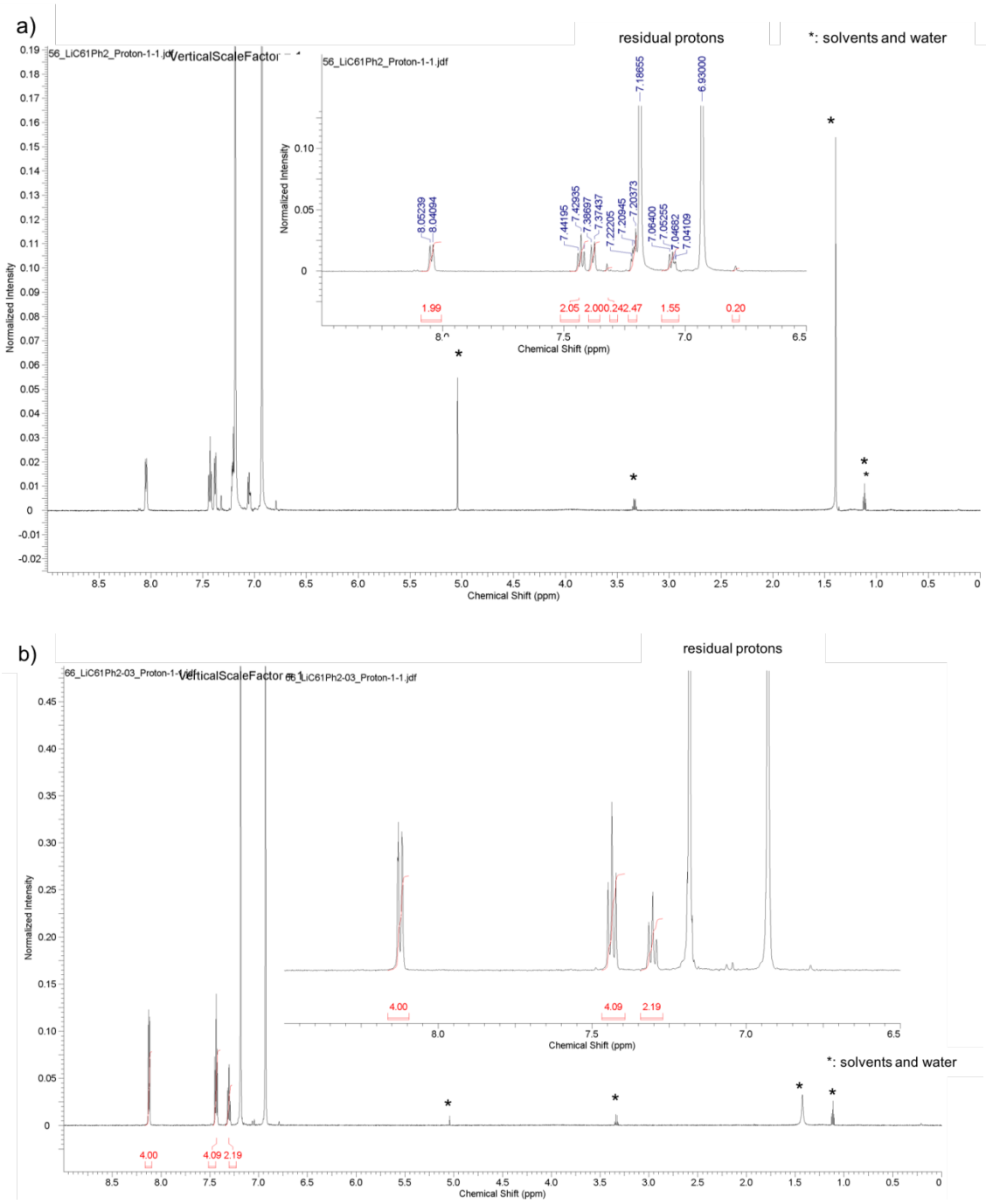


Figure S4. The ^{1}H NMR (600 MHz) spectra of [5,6]- and [6,6]- $[Li^{+}@C_{61}Ph_2]TFSI^{-}$ in 1,2-dichlorobenzene-d_4. (a) [5,6]-$[Li^{+}@C_{61}Ph_2]TFSI^{-}$. (b) [6,6]-$[Li^{+}@C_{61}Ph_2]TFSI^{-}$.

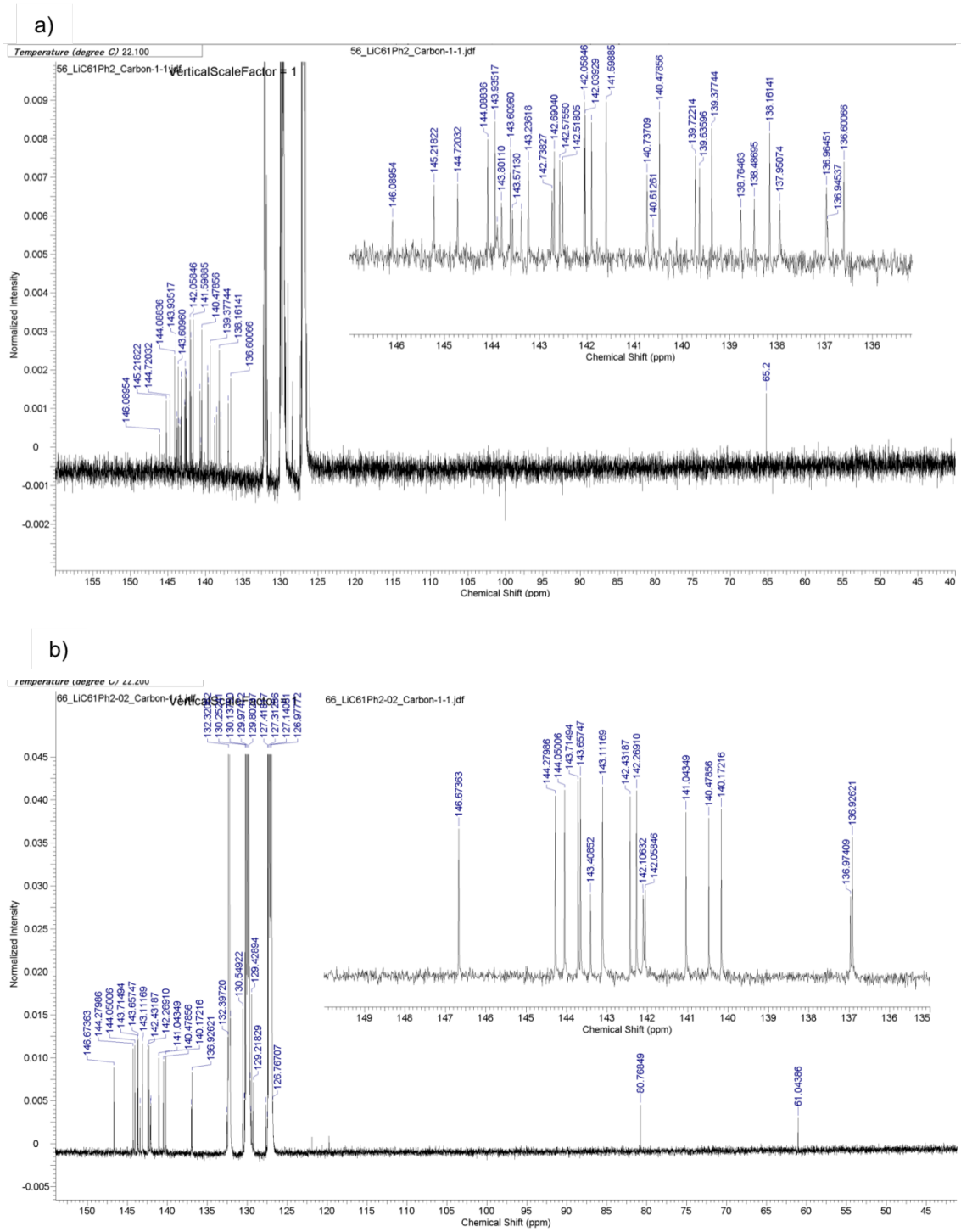


Figure S5. The ^{13}C NMR (151 MHz) spectra of [5,6]- and [6,6]- [Li^+@$C_{61}Ph_2$]$TFSI^-$ in 1,2-dichlorobenzene-d_4. (a) [5,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$. (b) [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$.

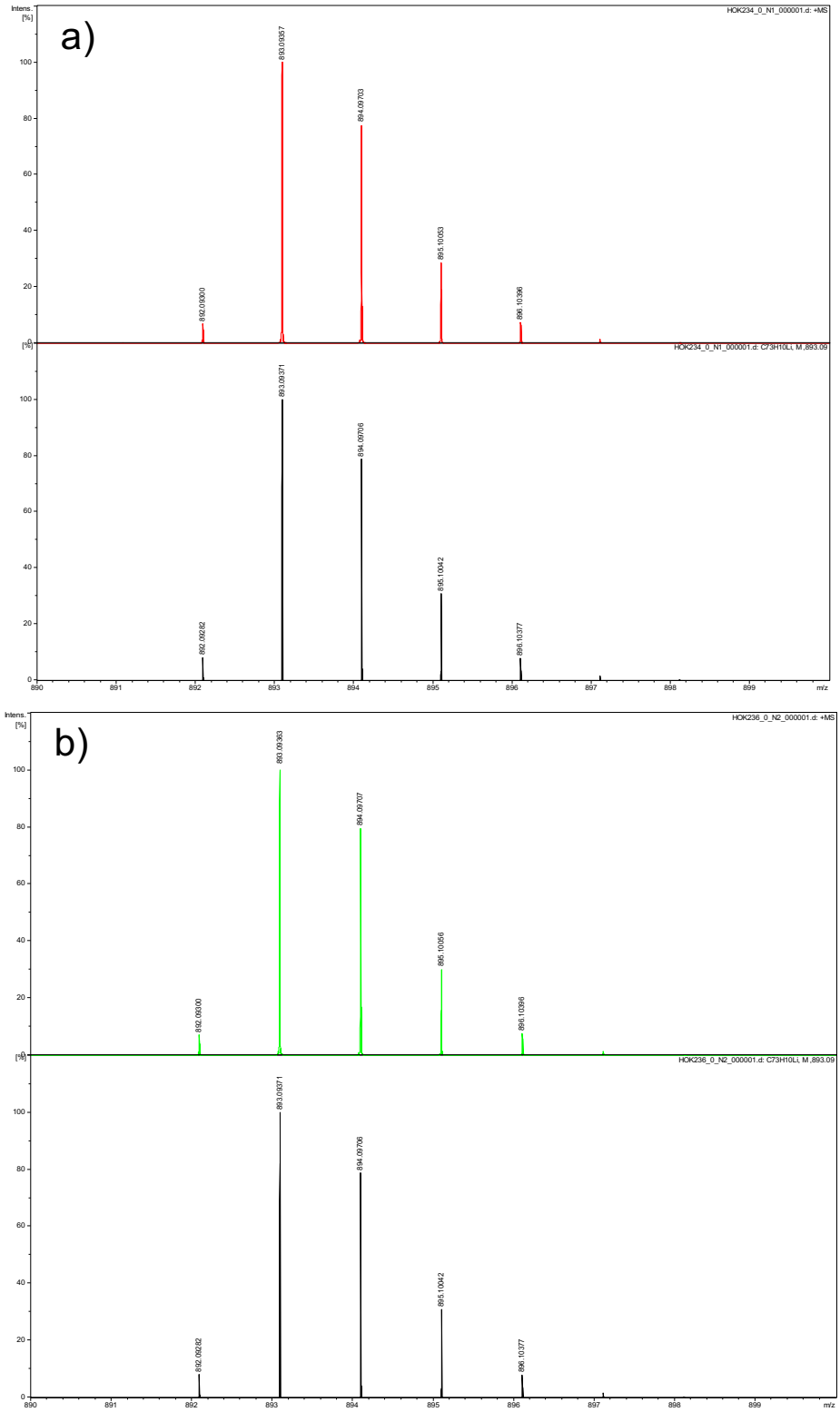


Figure S6. The MALDI-FT-ICR mass spectra of [5,6]- and [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$ for the cationic parts at the positive mode. Top, measured; Bottom, simulated. (a) [5,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$. (b) [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$.

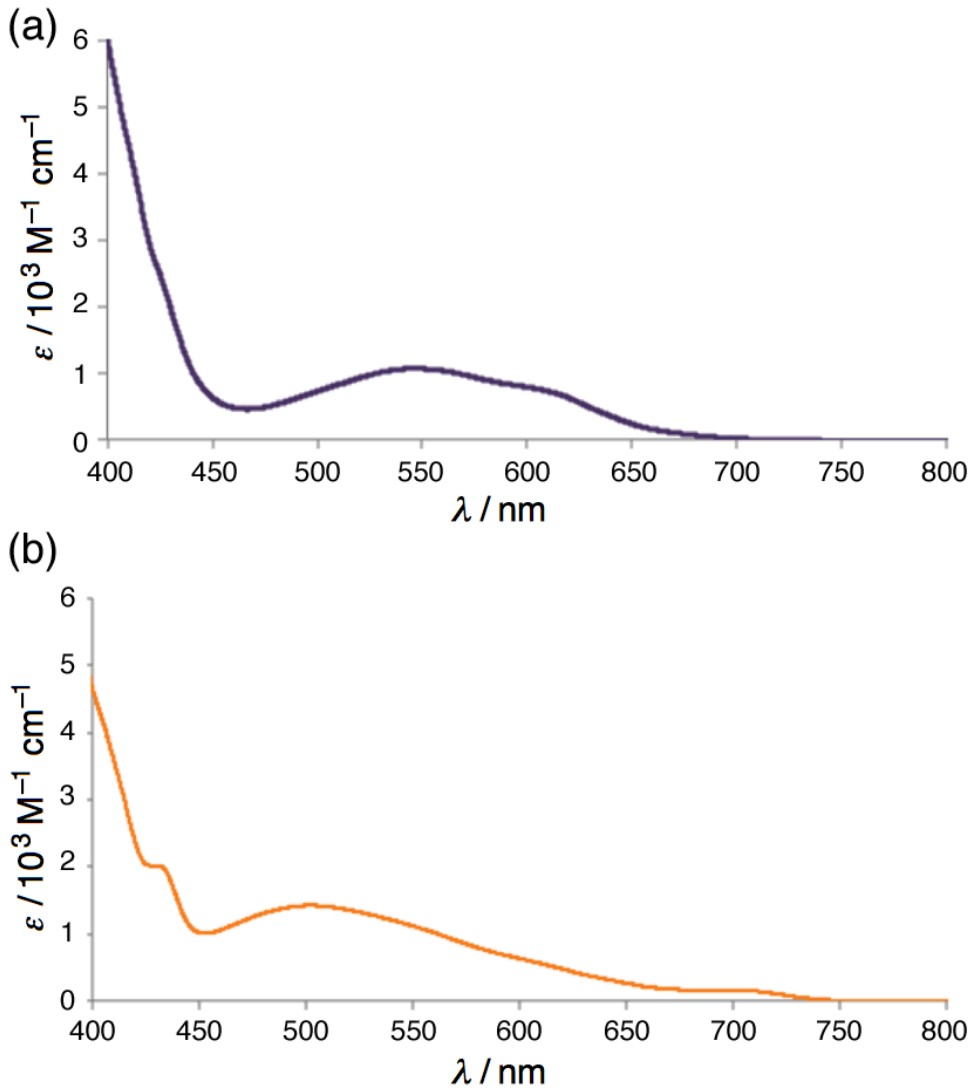


Figure S7. The UV-vis absorption spectra of [5,6]- and [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$ in CH_2Cl_2 solution. (a) [5,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$. (b) [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$.

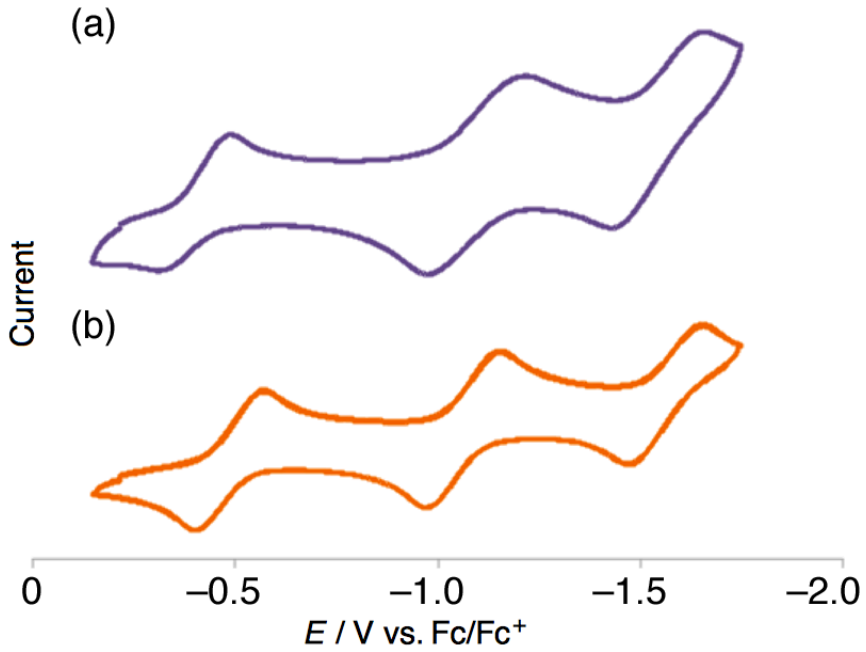


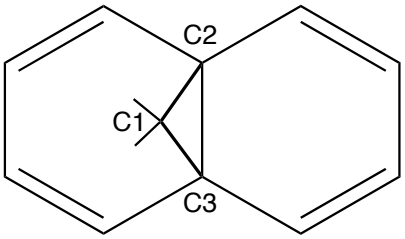
Figure S8. Cyclic voltammograms of [5,6]- and [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$ in 1,2-dichlorobenzene containing 50 mM *n*-Bu_4NPF_6 supporting electrolyte. Working electrode: glassy carbon. Counter electrode: Pt wire. Reference electrode: Ag/$AgNO_3$ in acetonitrile containing 100 mM *n*-Bu_4NClO_4. (a) [5,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$. (b) [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$.

Table S1. Reduction potentials of [5,6]- and [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$

	$E_{1/2}^{red1}$	$E_{1/2}^{red2}$	$E_{1/2}^{red3}$
	[V] vs. Fc^+/Fc		
[Li^+@C_{60}]	–0.43	–1.02	–1.49
[5,6]-[Li^+@$C_{61}Ph_2$]	–0.40	–1.10	–1.54
[6,6]-[Li^+@$C_{61}Ph_2$]	–0.49	–1.07	–1.57

Table S2. Bond lengths (Å) at the three-membered rings of [6,6]-methano[60]fullerenes

Compound	C2–C3	C1–C2	C1–C3	reported year	CCDC No.	ref.
PCBM·(*o*-DCB)	1.625(3)	1.518(4)	1.517(3)	2003	211976	1
PCBM·0.5(chlorobenzene)	1.630(3)	1.501(4)	1.514(3)	2003	211977	1
idem (another independent molecule)	1.625(3)	1.515(3)	1.525(3)	2003	211977	1
Li^+@PCBM	1.80(4)	1.59(4)	1.65(4)	2012	876699	2
$C_{61}Ph\{2,3\text{-}(MeO)_2C_6H_3\}\cdot 2$(chloroform)	1.614(7)	1.510(7)	151.5(7)	1994	—	3
$C_{61}(4\text{-}MeOC_6H_5)_2$	1.635(4)	1.514(4)	1.516(4)	1996	126496	4
$C_{61}(4\text{-}BrC_6H_5)_2$	1.76(3)	1.48(2)	1.42(2)	1998	—	5
$C_{61}(COOEt)_2\cdot$(chloroform)	1.607(4)	1.516(4)	1.510(4)	1995	1207279	6
idem (another independent molecule)	1.605(4)	1.509(4)	1.519(4)	1995	1207279	6
$C_{61}(C{\equiv}CC{\equiv}CSiMe_3)_2\cdot 0.5(CS_2)$	1.575(9)	1.527(8)	1.530(7)	1994	1174857	7
$C_{61}(C{\equiv}CC{\equiv}CSiMe_3)_2\cdot 2$(toluene)	1.574(2)	1.535(2)	1.543(2)	1994	1174858	7
$C_{60}(C_{19}H_{42}S_2Si_4)\cdot 2(CS_2)$	1.634(10)	1.553(10)	1.518(10)	2005	281589	8
$C_{61}Cl(CH_2Ph)\cdot 0.5(CS_2)$	1.637(16)	1.55(2)	1.525(12)	2007	622039	9
idem (another independent molecule)	1.602(10)	1.534(12)	1.480(10)	2007	622039	9
$C_{61}Ph(CF_3)\cdot 0.5(CS_2)$	1.588(4)	1.526(4)	1.527(3)	2007	643420	10
idem (another independent molecule)	1.634(3)	1.511(3)	1.524(4)	2007	643420	10



References for Table S2

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Table S3. Crystallographic data for [5,6]- and [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$

compound	[5,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$	[6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$
formula	$(LiC_{73}H_{10})(NC_2S_2O_4F_6)(C_6H_5Cl)_{0.77}$	$(LiC_{73}H_{10})(NC_2S_2O_4F_6)(C_6H_5Cl_2)_{0.92}$
formula weight	1260.67	1308.84
crystal size (mm)	0.12 × 0.02 × 0.01	0.10 × 0.10 × 0.02
temperature	100 K	100 K
X-ray wavelength	0.41289 Å	0.41285 Å
crystal system	triclinic	monoclinic
space group	$P\bar{1}$	$C2/m$
unit cell parameters	a = 10.377(1) Å	a = 27.1856(5) Å
	b = 14.517(1) Å	b = 10.4470(6) Å
	c = 18.313(2) Å	c = 21.7625(5) Å
	α = 85.74(1)°	β = 126.740(2) °
	β = 72.95(1)°	V = 4953.0(3) $Å^3$
	γ = 68.68(1)°	
	V = 2455.4(5) $Å^3$	
Z	2	4
No. of independent reflections	5,287 (d > 0.70 Å, $\|F\| > 3\sigma$)	7,225 (d > 0.60 Å, $\|F\| > 3\sigma$)
$\Sigma\sigma_I/\Sigma I$	0.0554	0.0471
No. of parameters	1107	515
$R1$	0.0660 ($\|F\| > 3\sigma$)	0.0735 ($\|F\| > 3\sigma$)
GOF	1.077 ($\|F\| > 3\sigma$)	1.59 ($\|F\| > 3\sigma$)

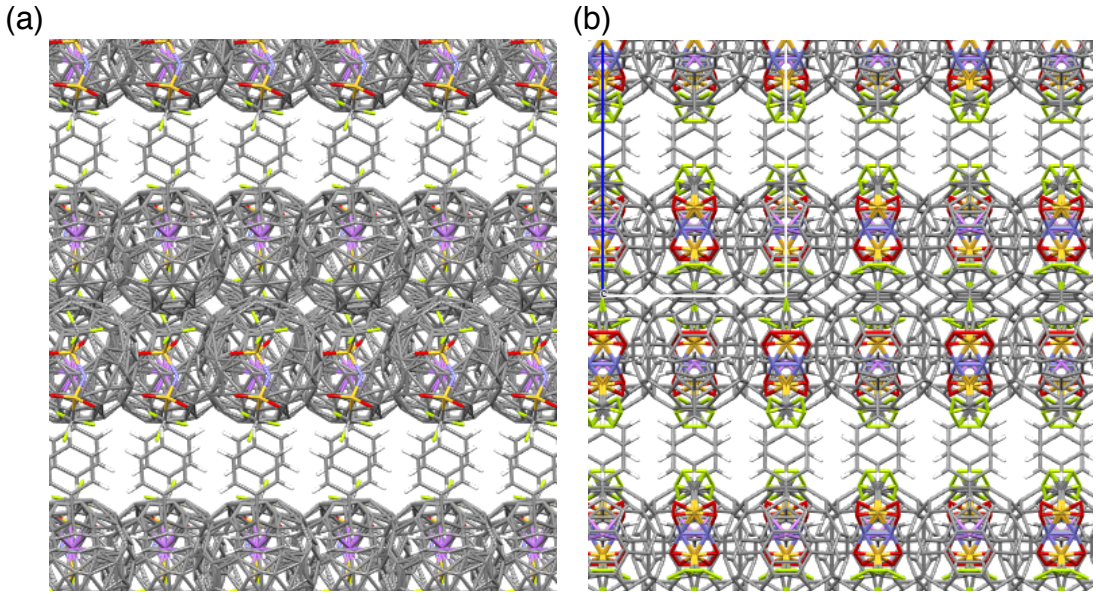
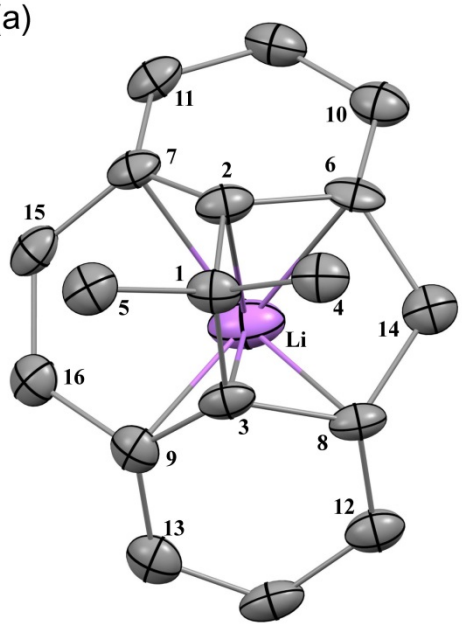


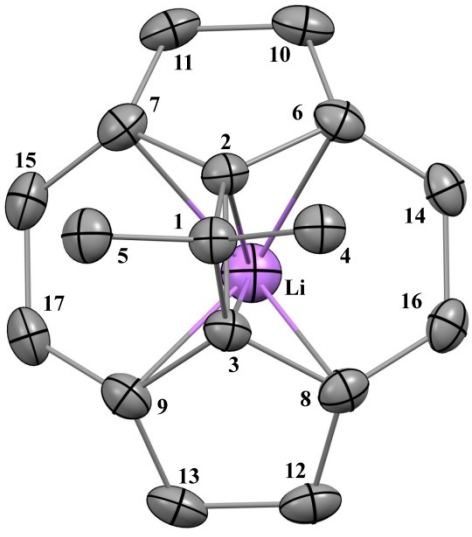
Figure S9. Crystal packing structures of [5,6]- and [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$. Crystal solvents were omitted for clarity. (a) The packing structure of [5,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$ in the view from the axis (corresponds to *a* axis of the structure of [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$) which is perpendicular to *a* axis of [5,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$. (b) The packing structure of [6,6]-[Li^+@$C_{61}Ph_2$]$TFSI^-$ in the view from the *a* axis. The Ph groups were ordered in the *a*-*c* plane.

(a)



2–3:	2.131(8)
1–2:	1.507(6)
1–3:	1.511(6)
1–4:	1.537(7)
1–5:	1.531(7)
2–6:	1.536(11)
2–7:	1.363(11)
3–8:	1.529(11)
3–9:	1.358(11)
6–10:	1.413(12)
6–14:	1.484(10)
7–11:	1.455(12)
7–15:	1.471(11)
8–12:	1.410(12)
8–14:	1.486(11)
9–13:	1.445(12)
9–16:	1.476(11)
15–16:	1.408(13)
Li–2:	2.391(10)
Li–3:	2.381(10)
Li–6:	2.301(18)
Li–7:	2.355(18)
Li–8:	2.332(19)
Li–9:	2.33(2)

(b)



2–3:	1.696(4)
1–2:	1.505(3)
1–3:	1.505(3)
1–4:	1.518(4)
1–5:	1.511(4)
2–6:	1.492(3)
2–7:	1.491(3)
3–8:	1.492(3)
3–9:	1.491(3)
6–10:	1.452(3)
6–14:	1.388(3)
7–11:	1.441(3)
7–15:	1.392(3)
8–12:	1.452(3)
8–16:	1.388(3)
9–13:	1.441(3)
9–17:	1.392(3)
14–16:	1.479(4)
15–17:	1.471(5)
Li–2:	2.299(6)
Li–3:	2.299(6)
Li–6:	2.368(5)
Li–7:	2.406(5)
Li–8:	2.368(5)
Li–9:	2.406(5)

Figure S10. *ORTEP* figures and bond lengths in Angstrom unit around the central carbon atoms of the attached CPh_2 group for (a) the major [5,6]-isomer and (b) the [6,6]-isomer. The thermal ellipsoids are shown at the 50% probability level.

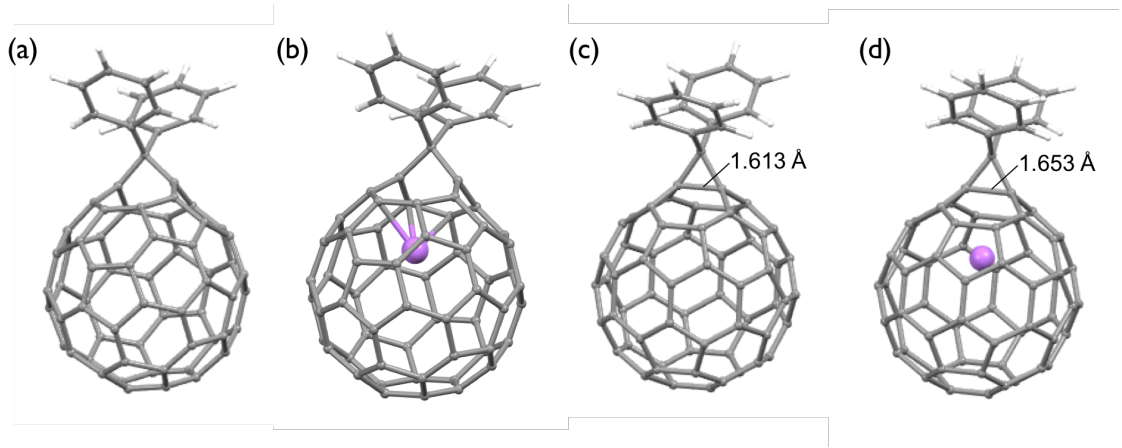


Figure S11. The optimized structures of empty and Li^+-containing $C_{61}Ph_2$. (a) [5,6]-$C_{61}Ph_2$. (b) [5,6]-[Li^+@$C_{61}Ph_2$]. (c) [6,6]-$C_{61}Ph_2$. (d) [6,6]-[Li^+@$C_{61}Ph_2$]. Calculations were carried out by using Gaussian09 package at the B3LYP. Solvent effects were estimated by the polarizable continuum model (PCM) method with the dielectric constant for *o*-dichlorobenzene. A 6-31G(d) basis set was used for each level.

Table S4. Calculated the energies and the numbers of imaginary frequency for the optimized structures

Compound	Gibbs Energy (Hartree)	number of imaginary frequency
[5,6]-$C_{61}Ph_2$	-2787.050363	0
[6,6]-$C_{61}Ph_2$	-2787.065219	0
[5,6]-[Li^+@$C_{61}Ph_2$]	-2794.465292	0
[6,6]-[Li^+@$C_{61}Ph_2$]	-2794.478063	0

Table S5. Calculated relative Gibbs energies of the [5,6]-isomers compared with the [6,6]-isomers

Compound	ΔG (kcal/mol [kJ/mol])
[5,6]-$C_{61}Ph_2$	9.36 [38.6]
[6,6]-$C_{61}Ph_2$	0
[5,6]-[Li^+@$C_{61}Ph_2$]	8.05 [33.2]
[6,6]-[Li^+@$C_{61}Ph_2$]	0

Table S6. Cartesian coordinates for the optimized structures

1. [5,6]-$C_{61}Ph_2$

Symbol	X	Y	Z
C	0.048020	-0.018693	-0.081884
C	0.008865	-0.032345	1.318995
H	0.933557	-0.050065	1.887112
C	-1.209614	-0.026462	1.999757
H	-1.215974	-0.041580	3.086254
C	-2.411759	0.000316	1.290562
H	-3.360594	0.002802	1.819814
C	-2.383228	0.029845	-0.104802
H	-3.310824	0.058877	-0.670002
C	-1.163853	0.023756	-0.784227
H	-1.161205	0.049747	-1.869356
C	1.711070	1.587858	-0.964237
C	1.226860	2.321292	-2.054554
H	0.678641	1.816909	-2.845179
C	1.444022	3.697548	-2.139628
H	1.064143	4.248801	-2.995491
C	2.145868	4.362002	-1.131684
H	2.317097	5.432778	-1.198253
C	2.625018	3.639441	-0.037056
H	3.170709	4.145068	0.754959
C	2.406925	2.263199	0.046211
H	2.784986	1.713605	0.903549
C	1.388498	0.089631	-0.825013
C	1.481136	-0.679828	-2.120570
C	2.518683	-0.728768	-0.249542
C	2.657311	-0.431916	-2.962685
C	0.830025	-1.906582	-2.313783
C	2.309647	-1.975851	0.355742
C	3.861363	-0.488292	-0.789721
C	0.891203	-2.537225	-3.611203
C	2.697721	-1.020042	-4.230313
C	0.667421	-2.968073	-1.313948
C	1.352535	-2.999828	-0.077243
C	3.922021	-0.218838	-2.237008
C	4.943898	-1.123586	-0.174606
C	3.427046	-2.655029	0.967160
C	0.513565	-4.225708	-2.061956

C	5.127860	-0.511710	-2.912229
C	1.876823	-4.288902	0.400671
C	0.635713	-3.947817	-3.477723
C	1.749105	-2.058770	-4.593280
C	1.243853	-4.852372	-4.348254
C	1.763458	-6.103578	-3.832590
C	0.997678	-5.437944	-1.578373
C	1.637097	-6.390937	-2.473431
C	5.137749	-1.047143	-4.263515
C	3.936892	-1.311773	-4.906678
C	6.266335	-1.099432	-2.225440
C	6.167946	-1.415332	-0.877748
C	4.818024	-3.434823	-5.795585
C	6.083880	-3.156016	-5.137308
C	3.767888	-2.525256	-5.689714
C	6.242160	-1.983987	-4.394518
C	6.942592	-2.016927	-3.128067
C	6.610744	-4.411458	-4.630950
C	7.286543	-4.442543	-3.409784
C	7.462974	-3.219631	-2.645997
C	2.159687	-4.365340	-5.366773
C	3.253554	-5.315669	-5.472516
C	2.410950	-2.996018	-5.482273
C	4.556376	-4.860273	-5.686217
C	5.664654	-5.463887	-4.965308
C	3.006656	-6.393523	-4.527449
C	4.070919	-6.973093	-3.836349
C	5.427300	-6.500980	-4.061516
C	7.080253	-4.976955	-1.127729
C	7.044419	-5.527039	-2.472425
C	6.130942	-6.533338	-2.790850
C	6.197400	-5.451663	-0.155273
C	5.808835	-3.153063	0.654217
C	6.715341	-2.661380	-0.366654
C	7.343278	-3.551597	-1.235447
C	5.547873	-4.521970	0.752829
C	3.147379	-4.064262	1.057664
C	4.724825	-2.196436	0.780408
C	4.188034	-4.988607	0.969664
C	2.775321	-6.443647	-0.417595
C	1.697696	-5.470843	-0.312748

C	3.999993	-6.207487	0.207321
C	5.209755	-7.025632	-1.779657
C	3.934405	-7.291761	-2.424696
C	2.741171	-7.005162	-1.756700
C	5.242240	-6.496467	-0.489379

2. [6,6]-$C_{61}Ph_2$

Symbol	X	Y	Z
C	0.002721	-0.015099	-0.039386
C	0.004460	-0.013986	1.477628
C	1.213936	-0.024947	2.184616
H	2.154884	0.035097	1.644987
C	1.220930	-0.110039	3.577718
H	2.167339	-0.115184	4.111320
C	0.017303	-0.185821	4.282117
H	0.022245	-0.249552	5.366643
C	0.054437	-1.416770	-0.617154
C	-1.127766	-2.135703	-0.837650
H	-2.088790	-1.662155	-0.657750
C	-1.081983	-3.455050	-1.290249
H	-2.007840	-3.998034	-1.458961
C	0.147830	-4.073320	-1.526910
H	0.183737	-5.099761	-1.881036
C	0.766133	1.084100	-0.753572
C	1.357480	2.308021	-0.131005
C	1.414388	0.993385	-2.097624
C	0.606019	3.258504	0.542345
C	0.716324	0.714448	-3.262037
C	2.477535	2.734107	-0.934544
C	2.512668	1.928060	-2.139739
C	2.869825	4.074545	-0.979199
C	2.939206	2.492177	-3.345141
C	2.105914	5.060441	-0.252481
C	2.230782	2.177885	-4.563014
C	0.985778	4.655915	0.481474
C	1.130774	1.315158	-4.514322
C	-0.223730	5.458537	0.447510
C	-0.057242	1.621239	-5.291004
C	3.302291	4.664866	-2.235271
C	3.335794	3.889971	-3.393841
C	2.796464	6.025399	-2.283220

C	2.864792	4.440762	-4.652320
C	2.055409	6.269483	-1.055907
C	2.180586	3.380839	-5.375628
C	0.890327	7.036883	-1.087889
C	1.036340	3.672608	-6.119221
C	-0.271062	6.625998	-0.315465
C	-0.103729	2.771049	-6.080453
C	2.340710	6.555859	-3.491710
C	2.375679	5.747658	-4.700071
C	1.128920	7.356023	-3.522013
C	1.185600	6.049207	-5.476058
C	0.419464	7.592506	-2.342930
C	0.530533	5.031702	-6.172774
C	0.415244	7.044713	-4.749369
C	-1.198337	-0.092644	2.191348
H	-2.144315	-0.085531	1.657330
C	-1.192555	-0.177376	3.584676
H	-2.134168	-0.235094	4.123634
C	1.283807	-2.044719	-0.854552
H	2.208783	-1.500012	-0.687728
C	-0.845120	1.018316	-0.755220
C	-1.537048	2.189072	-0.134914
C	-1.479732	0.874007	-2.101083
C	-0.868443	3.197735	0.540564
C	-0.758132	0.653658	-3.263701
C	-2.686883	2.520312	-0.940936
C	-2.651995	1.713888	-2.146067
C	-3.188898	3.823682	-0.986647
C	-3.120404	2.240827	-3.352718
C	-2.510473	4.869146	-0.258473
C	-2.385498	1.986490	-4.568836
C	-1.362709	4.558797	0.478639
C	-1.217723	1.218076	-4.517051
C	-3.665054	4.375832	-2.244181
C	-3.631461	3.600804	-3.402688
C	-3.273553	5.773661	-2.290929
C	-3.203980	4.189119	-4.659765
C	-2.558123	6.078310	-1.061894
C	-2.432794	3.189422	-5.381485
C	-1.460608	6.939508	-1.090821
C	-1.314556	3.575004	-6.121971

C	-2.860246	6.340278	-3.498269
C	-2.824826	5.531878	-4.706399
C	-1.719045	7.238115	-3.525604
C	-1.662245	5.931030	-5.479778
C	-1.034337	7.532361	-2.344774
C	-0.923219	4.971228	-6.174390
C	-0.978902	6.986993	-4.751189
C	1.330842	-3.364344	-1.307204
H	2.292329	-3.836393	-1.489215

3. [5,6]-[Li^{+}@$C_{61}Ph_2$]

Symbol	X	Y	Z
Li	-0.210666	-0.069583	-0.336651
C	-0.047434	0.017933	4.203865
C	1.218210	-0.029383	4.803903
H	2.045323	0.531241	4.379821
C	1.433753	-0.793679	5.951513
H	2.423671	-0.820196	6.398155
C	0.384954	-1.516434	6.522569
H	0.553136	-2.113195	7.414445
C	-0.883275	-1.460293	5.942086
H	-1.710678	-2.009760	6.381990
C	-1.098700	-0.695939	4.794131
H	-2.094178	-0.658465	4.362584
C	-0.708095	2.323640	3.548995
C	-2.046804	2.613451	3.839615
H	-2.822206	1.884080	3.622324
C	-2.398447	3.836344	4.413644
H	-3.441971	4.046503	4.630156
C	-1.415185	4.782410	4.709788
H	-1.688785	5.734158	5.156005
C	-0.077220	4.495836	4.431487
H	0.697107	5.222231	4.661399
C	0.274083	3.273477	3.857077
H	1.319886	3.063013	3.651581
C	-0.308021	0.942359	3.004960
C	-1.250486	0.397015	1.956520
C	0.798191	0.993357	1.976586
C	-1.695509	1.324240	0.899696
C	-1.326280	-0.977731	1.652119
C	1.609767	-0.117774	1.684540

C	0.697831	2.019187	0.928029
C	-2.321165	-1.435270	0.705540
C	-2.675089	0.881162	-0.003275
C	-0.197204	-1.921761	1.600473
C	1.163147	-1.516177	1.608310
C	-0.667034	2.275253	0.421388
C	1.783952	2.181191	0.059244
C	2.724916	0.039379	0.775325
C	-0.601213	-3.012329	0.692442
C	-0.799335	2.785470	-0.893252
C	2.109235	-2.204143	0.715616
C	-1.913536	-2.706199	0.155305
C	-3.045386	-0.526677	-0.063726
C	-2.260378	-3.036949	-1.155359
C	-1.291344	-3.698262	-2.007645
C	0.320194	-3.651701	-0.134909
C	-0.027486	-4.003720	-1.503373
C	-1.883474	2.369694	-1.774086
C	-2.801556	1.421120	-1.339022
C	0.359635	3.021765	-1.738812
C	1.630681	2.710241	-1.273980
C	-2.747338	0.288303	-3.527219
C	-1.796973	1.285967	-3.990680
C	-3.241949	0.355999	-2.226909
C	-1.382025	2.310316	-3.138354
C	0.006990	2.716818	-3.117466
C	-0.837834	0.625124	-4.858500
C	0.501865	1.018701	-4.839790
C	0.931149	2.088486	-3.954193
C	-3.000238	-2.084664	-1.969803
C	-2.485128	-2.159205	-3.325848
C	-3.382862	-0.853003	-1.435940
C	-2.363006	-0.995998	-4.090958
C	-1.182320	-0.787061	-4.911523
C	-1.430864	-3.160219	-3.351000
C	-0.297501	-2.959548	-4.140067
C	-0.172000	-1.749642	-4.935131
C	2.635829	0.466679	-4.016309
C	1.552724	0.013413	-4.871520
C	1.222175	-1.341653	-4.916614
C	3.348546	-0.450549	-3.243090

C	3.354512	1.120031	-1.339959
C	2.604216	2.068333	-2.143428
C	2.254054	1.750800	-3.453657
C	3.711649	-0.119253	-1.875802
C	3.078272	-1.245735	0.223737
C	2.860694	1.202145	0.021961
C	3.577491	-1.327101	-1.076135
C	2.231007	-3.346507	-1.472716
C	1.710556	-3.245502	-0.116472
C	3.143309	-2.402856	-1.947589
C	1.960456	-2.298566	-4.108324
C	1.020205	-3.295868	-3.622881
C	1.150983	-3.805155	-2.329380
C	3.002325	-1.862676	-3.289544

4. [6,6]-[Li^{+}@$C_{61}Ph_2$]

Symbol	X	Y	Z
Li	-0.072916	0.000000	-0.317853
C	-0.040572	0.000000	3.365596
C	1.227466	0.000000	4.199578
C	1.789363	-1.208067	4.631191
H	1.356442	-2.152075	4.311658
C	2.901098	-1.207830	5.474704
H	3.328536	-2.151846	5.800684
C	3.460225	0.000000	5.897710
H	4.326202	0.000000	6.553591
C	-1.297049	0.000000	4.216786
C	-1.852828	1.208051	4.656319
H	-1.424107	2.152166	4.331548
C	-2.952818	1.207802	5.515114
H	-3.375502	2.151837	5.847178
C	-3.506130	0.000000	5.945748
H	-4.363092	0.000000	6.613366
C	-0.048712	-0.826384	2.097632
C	1.131545	-1.461481	1.431969
C	-1.237930	-1.461374	1.448015
C	2.232036	-0.740023	0.981740
C	-2.344160	-0.739817	1.012942
C	0.668081	-2.603315	0.670341
C	-0.785869	-2.603648	0.680104

C	1.360020	-3.043322	-0.461102
C	-1.494561	-3.044745	-0.440337
C	2.527105	-2.314139	-0.907529
C	-2.667732	-2.314590	-0.870481
C	2.944116	-1.177018	-0.205851
C	-3.075252	-1.177311	-0.163234
C	3.394796	0.000000	-0.930973
C	-3.534986	0.000000	-0.882411
C	0.623935	-3.501942	-1.629844
C	-0.774680	-3.501984	-1.619886
C	1.342155	-3.040516	-2.805868
C	-1.508925	-3.039774	-2.785533
C	2.520020	-2.311398	-2.360506
C	-2.680827	-2.311304	-2.323612
C	2.939276	-1.176230	-3.054617
C	-3.109535	-1.176041	-3.011816
C	3.392891	0.000000	-2.328162
C	-3.554193	0.000000	-2.279509
C	0.635762	-2.604227	-3.927698
C	-0.818582	-2.604178	-3.917516
C	1.078028	-1.424473	-4.651289
C	-1.271176	-1.424834	-4.635425
C	2.209777	-0.727454	-4.226230
C	-2.396373	-0.727447	-4.193496
C	-0.099752	-0.698433	-5.096713
C	1.789363	1.208067	4.631191
H	1.356442	2.152075	4.311658
C	2.901098	1.207830	5.474704
H	3.328536	2.151846	5.800684
C	-1.852828	-1.208051	4.656319
H	-1.424107	-2.152166	4.331548
C	-0.048712	0.826384	2.097632
C	1.131545	1.461481	1.431969
C	-1.237930	1.461374	1.448015
C	2.232036	0.740023	0.981740
C	-2.344160	0.739817	1.012942
C	0.668081	2.603315	0.670341
C	-0.785869	2.603648	0.680104
C	1.360020	3.043322	-0.461102
C	-1.494561	3.044745	-0.440337
C	2.527105	2.314139	-0.907529

C	-2.667732	2.314590	-0.870481
C	2.944116	1.177018	-0.205851
C	-3.075252	1.177311	-0.163234
C	0.623935	3.501942	-1.629844
C	-0.774680	3.501984	-1.619886
C	1.342155	3.040516	-2.805868
C	-1.508925	3.039774	-2.785533
C	2.520020	2.311398	-2.360506
C	-2.680827	2.311304	-2.323612
C	2.939276	1.176230	-3.054617
C	-3.109535	1.176041	-3.011816
C	0.635762	2.604227	-3.927698
C	-0.818582	2.604178	-3.917516
C	1.078028	1.424473	-4.651289
C	-1.271176	1.424834	-4.635425
C	2.209777	0.727454	-4.226230
C	-2.396373	0.727447	-4.193496
C	-0.099752	0.698433	-5.096713
C	-2.952818	-1.207802	5.515114
H	-3.375502	-2.151837	5.847178

Reference for computational calculation with Gaussian 09, Revision D.01:
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