Electronic Supplementary Information

Electrochemical Reduction of Cationic $Li^+@C_{60}$ to Neutral $Li^+@C_{60}^{\bullet-}$: Isolation and Characterisation of Endohedral [60]Fulleride

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General Procedure

$[Li^+@C_{60}](PF_6^-)$ was obtained from Idea International Corporation. All other reagents were commercially available and used without further purification. $[Li^+@C_{60}](TFSI^-)$ was prepared by the reported procedure.[1] Ionic conductivity measurement was performed using a HORIBA ES-51 under N_2 atmosphere. UV-vis-NIR spectra were recorded on a Shimadzu UV-1800 and JASCO V570 spectrometer. ESR spectra were measured on a JEOL JES-FA100. The ^{7}Li, ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded at 233.12 MHz, 599.85 MHz, 150.84 MHz, and 564.23 MHz, respectively on a Varian Unity Inova 600. YAZAWA CS-12Z constant current regulator was used for electrochemical synthesis of $Li@C_{60}$.

The $(Li@C_{60})_2$-Ni(OEP) co-crystal was grown by electrochemical reduction of $[Li^+@C_{60}](TFSI^-)$ in the presence of Ni(OEP) that is widely used as a co-crystallizing agent for endohedral fullerenes. Due to the much lower LOMO level of $Li^+@C_{60}$, than that of NiOEP, only the $Li@C_{60}$ was electrochemically reduced on the surface of anode. When ca. 5 eq of Ni(OEP) was added, fortunately, we found the product deposited on the surface of cathode with Ni(OEP) as a co-crystal. Both $[Li^+@C_{60}](TFSI^-)$ and $Li^+@C_{60}^{\bullet-}$, before and after the electrochemical reduction, respectively, may form complexes with Ni(OEP) prior to give the dimer co-crystal.
Ni(OEP) (6 mg, 10 μmol) was added to a deaerated dichloromethane solution (30 mL) of $[Li^+@C_{60}](TFSI^-)$ (2 mg, 2 μmol) under nitrogen. The solution was placed in an H-shaped cell, cooled to 263 K, and electrolysed using a Pt electrode at a constant current (0.3 μA). A purplish-black crystal was given in approximately three days, and the obtained crystal was used for the X-ray structure analysis.

The X-ray diffraction data were collected by using the large cylindrical image-plate camera at SPring-8 BL02B1. The initial structure model was derived by a direct method using *SIR*. The structure refinement and modification were performed by using *SHELX* and *ENIGMA*. The results of the crystal structure analysis of the $Li^+@C_{60}^{\bullet-}$–Ni(OEP) co-crystal at 250 and 100 K are summarized in Table S1. The crystal information file (CIF) is available from the Cambridge Crystallographic Data Centre (CCDC). The CIF deposition numbers are CCDC 1458690-1458691.

Reference

[1] H. Okada and Y. Matsuo, *Fuller. Nanotub. Carbonnanostruct.*, 2014, **22**, 262.

Table S1. Crystallographic data for the $Li^+@C_{60}^{\bullet-}$–Ni(OEP) co-crystal.

formula	$(LiC_{60})_2(NiN_4C_{36}H_{44})_2(CCl_2H_2)_2$	$(LiC_{60})_2(NiN_4C_{36}H_{44})_2(CCl_2H_2)_2$
formula weight	2807.9	2807.9
color of crystal	Black	Black
temperature	250 K	100 K
X-ray wavelength	0.41286 Å	0.41286 Å
crystal system	Monoclinic	Monoclinic
space group	*C*2/*m*	$P2_1/a$
unit cell parameters	*a* = 24.505(1) Å *b* = 14.950(2) Å *c* = 17.435(1) Å β = 108.799(3) ° *V* = 6046.6(9) Å^3	*a* = 24.400(1) Å *b* = 14.864(1) Å *c* = 17.233(1) Å β = 108.543(3) ° *V* = 5925.6(6) Å^3
Z	2	2
No. of independent reflections	4,915 (*d* > 0.70 Å, $\|F\| > 3\sigma$)	10,513 (*d* > 0.65 Å, $\|F\| > 3\sigma$)
$\Sigma\sigma_I / \Sigma I$	0.0789	0.0690
No. of parameters	640	1003
*R*1	0.0644 ($\|F\| > 3\sigma$)	0.0624 ($\|F\| > 3\sigma$)
GOF	0.854 ($\|F\| > 3\sigma$)	0.964 ($\|F\| > 3\sigma$)

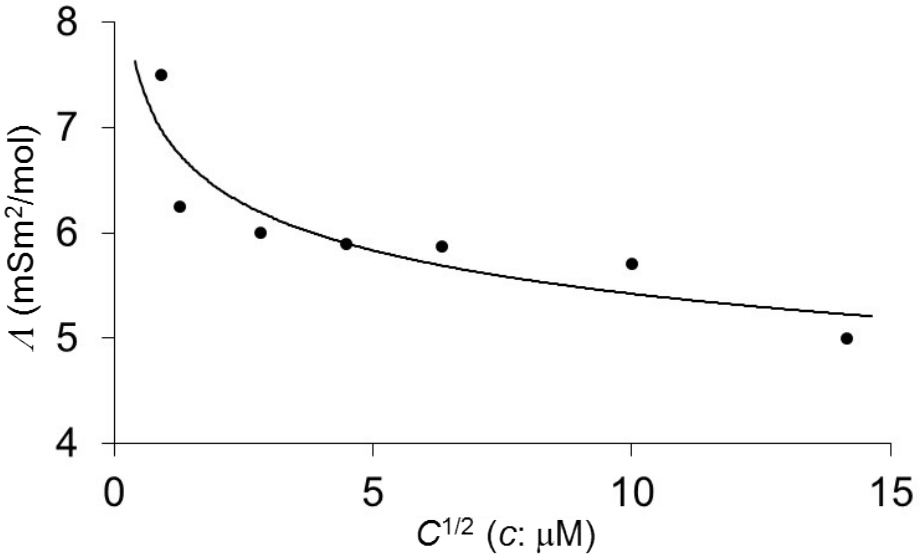


Fig. S1 Molar conductivity of $[Li^+@C_{60}](TFSI^-)$ measured in dichloromethane containing various concentrations of $[Li^+@C_{60}](TFSI^-)$ at 298 K.

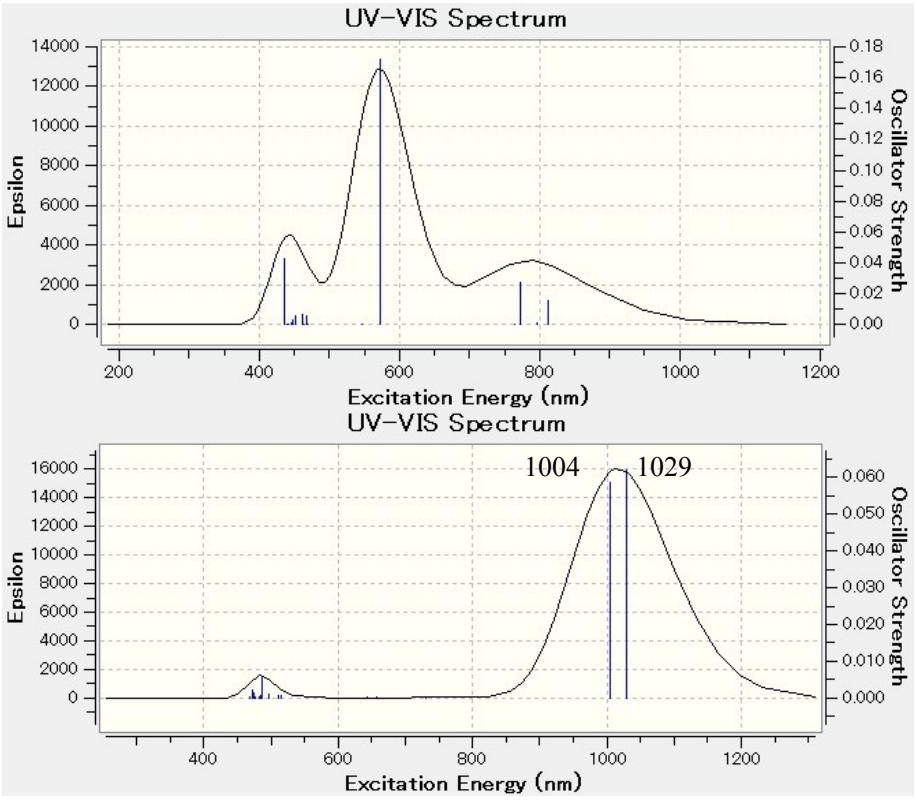


Fig. S2 Vis-NIR absorption spectra of $Li@C_{60}$ dimer (a) and $Li@C_{60}$ monomer (b) obtained by time-dependent (TD) DFT calculations (nstates = 20, wB97XD/6-31G(d)/IEFPCM).

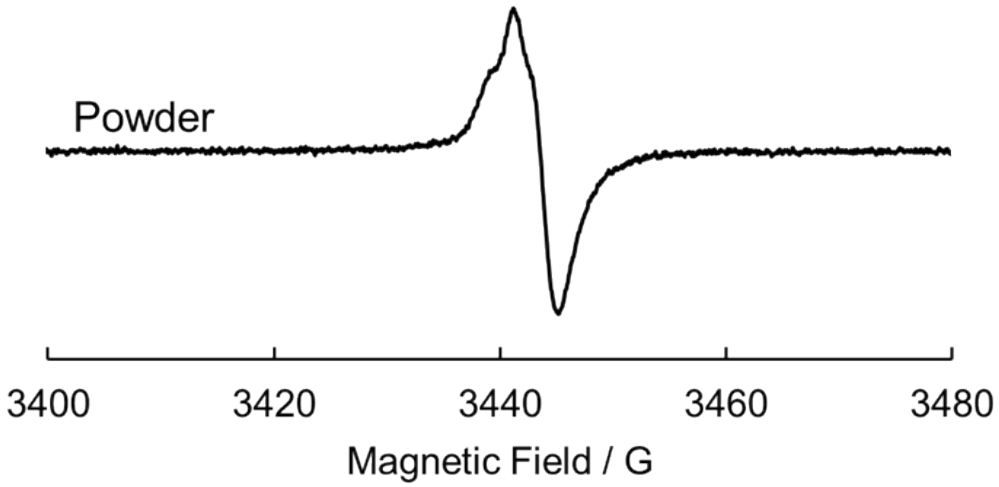


Fig. S3 ESR spectrum of the product measured for the collected powder sample of $Li^{+}@C_{60}^{\bullet-}$ at 77 K.

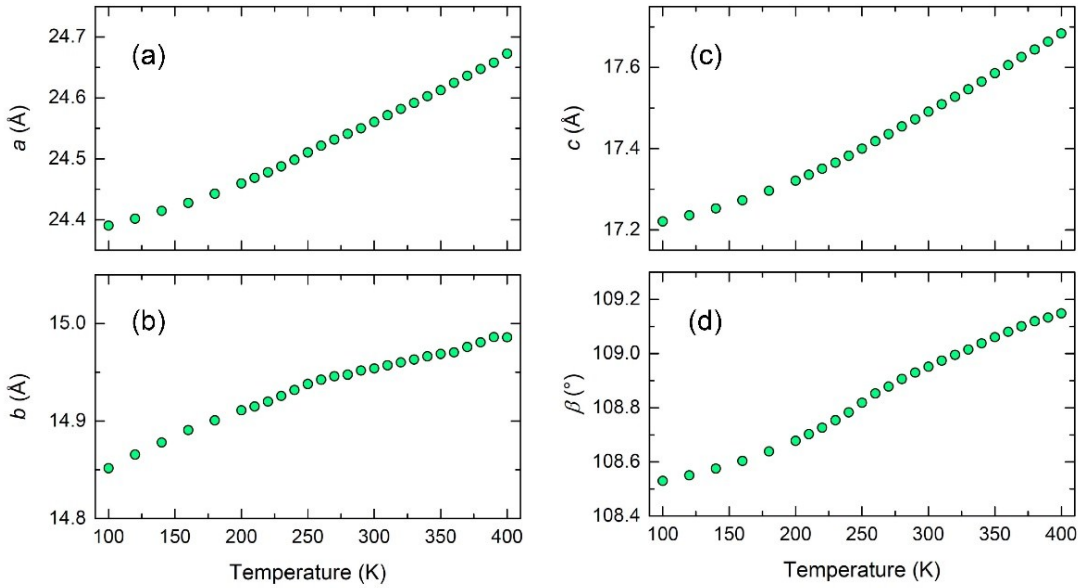
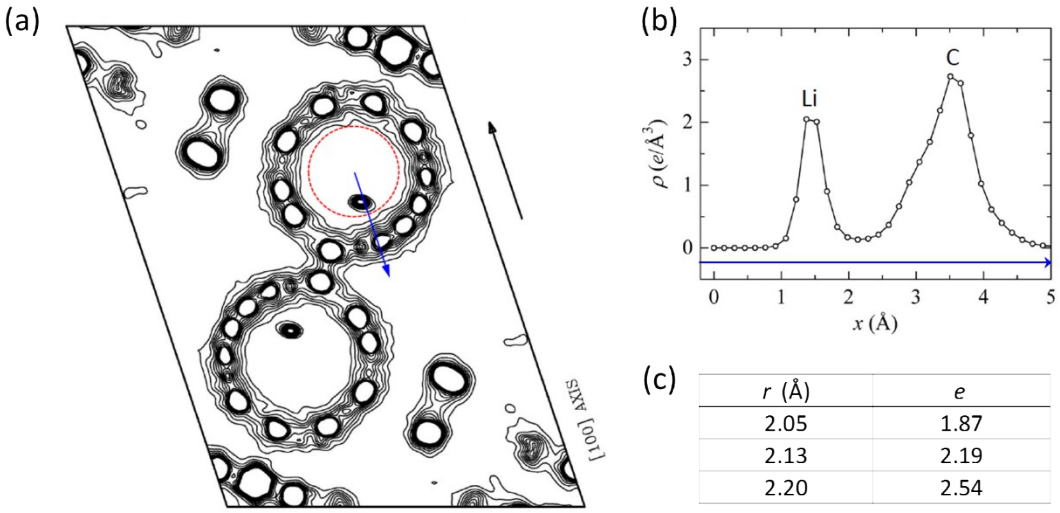


Fig. S4 Lattice constants and phase transition of the $Li^{+}@C_{60}^{\bullet-}$–Ni(OEP) co-crystal. a, b, c, d: The temperature dependence of the monoclinic lattice constants *a*, *b*, *c* and β, respectively.



(c)

r (Å)	*e*
2.05	1.87
2.13	2.19
2.20	2.54

Fig. S5 (a) MEM charge-density contour map of the $(Li@C_{60})_2$-Ni(OEP) co-crystal at 100 K. (b) MEM charge density profile on the blue arrow in (a). (c) Numbers of electrons inside the C_{60} which were estimated by counting electrons inside a sphere with the radius *r* (the red circle in (a)).

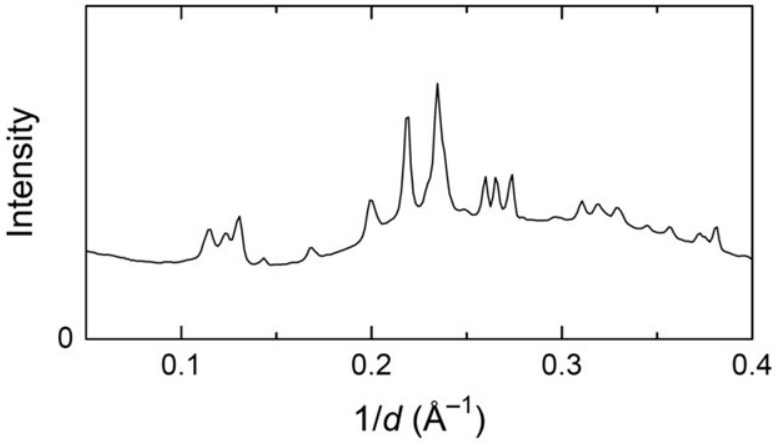


Fig. S6 X-ray diffraction pattern of the powder sample of $Li^+@C_{60}^{\bullet-}$ sealed into a glass capillary.

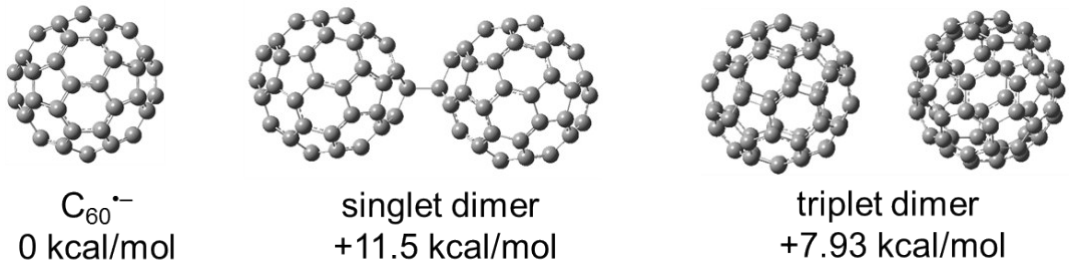


Fig. S7 Gibbs free energy differences between empty $C_{60}^{\bullet-}$ and its singlet/triplet dimers calculated by DFT calculation at M06-2X/6-31G(d) level of theory with SCRF (IEFPCM in *o*-DCB).

Table S2. List of Gibbs free energy differences (kcal/mol) between $Li^+@C_{60}^{\bullet-}$/$C_{60}^{\bullet-}$ and its singlet/triplet dimer estimated by theoretical calculation.

	$Li^+@C_{60}^{\bullet-}$		$C_{60}^{\bullet-}$	
	singlet	triplet	singlet	triplet
M06-2x/6-31G(d)/vac	-4.35	+6.19	+42.0	+36.9
M06-2x/6-31G(d)/IEFPCM	+0.29	+8.00	+11.5	+7.93
M06-2x/6-31G(d)/SMD	+1.77	+9.49	+15.5	+13.0
wB97XD/6-31G(d)/vac	-13.5	+1.85	+33.0	+31.8
wB97XD/6-31G(d)/SMD	-5.13	+6.32	+6.88	+8.64

Computational Results

Full geometry optimizations followed by frequency calculations and TD-DFT have been carried out by using the M06-2X or wB97XD functional with the 6-31G(d) basis set and solvent parameters (IEFPCM or SMD) in Gaussian 09 software. All frequency calculations showed no imaginary frequency. Full citation is as follows:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Cartesian Coodinates

$Li^+@C_{60}^-$ (doublet) by UM06-2x/6-31G(d) without solvent parameters

E(UM062X) = −2292.99610440 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2292.663606 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.436660	1.174824	3.025567
2	6	0	0.706286	−0.000716	3.469196
3	6	0	1.433115	−1.176994	3.027624
4	6	0	2.602451	−0.722803	2.296609
5	6	0	2.603941	0.729951	2.302127
6	6	0	3.034114	−1.415833	−1.169215
7	6	0	3.480478	−0.693586	−0.002420
8	6	0	3.029349	−1.417244	1.174090
9	6	0	2.305653	−2.595201	0.732390
10	6	0	2.300611	−2.587767	−0.719485
11	6	0	−1.416025	1.172163	3.031552
12	6	0	−2.580931	0.728514	2.316798
13	6	0	−2.570924	−0.728429	2.302484
14	6	0	−1.402951	−1.181683	3.034155
15	6	0	−0.681272	−0.002567	3.473903
16	6	0	0.727040	−2.298669	−2.593016
17	6	0	1.179134	−3.019298	−1.412193
18	6	0	0.012286	−3.476039	−0.680956
19	6	0	−1.157031	−3.017632	−1.403890
20	6	0	−0.709051	−2.301143	−2.592643
21	6	0	1.434444	−1.168951	−3.024166
22	6	0	0.703658	0.004523	−3.459262
23	6	0	1.430129	1.184275	−3.019610
24	6	0	2.601020	0.730951	−2.293205
25	6	0	2.598596	−0.723419	−2.298629
26	6	0	0.731765	2.299582	2.598457
27	6	0	1.184172	3.025091	1.420876
28	6	0	0.014735	3.477952	0.694142
29	6	0	−1.155906	3.018606	1.422950
30	6	0	−0.709896	2.303593	2.603454
31	6	0	0.743411	−2.307023	2.608432
32	6	0	−0.707575	−2.309884	2.609578
33	6	0	−1.154017	−3.038377	1.439960
34	6	0	0.015055	−3.482940	0.712103
35	6	0	1.189981	−3.033669	1.434116
36	6	0	3.037723	1.423635	1.172832
37	6	0	3.482275	0.700834	0.004152
38	6	0	3.030592	1.423637	−1.170686
39	6	0	2.306561	2.602109	−0.725592
40	6	0	2.306431	2.595598	0.727189
41	6	0	0.738656	2.312034	−2.596100
42	6	0	−0.711392	2.317786	−2.594228
43	6	0	−1.156148	3.041459	−1.425354
44	6	0	0.014387	3.486216	−0.696148
45	6	0	1.189722	3.038810	−1.421843
46	6	0	−3.484606	−0.711200	0.002246
47	6	0	−3.043034	−1.431408	−1.161601
48	6	0	−2.285436	−2.597679	−0.708310
49	6	0	−2.282583	−2.605600	0.742326
50	6	0	−3.007547	−1.429926	1.184224
51	6	0	−2.284711	2.608854	−0.722217
52	6	0	−3.008574	1.430048	−1.164150
53	6	0	−3.479954	0.705738	0.016928
54	6	0	−3.018549	1.420444	1.176219
55	6	0	−2.281256	2.595234	0.725834
56	6	0	−1.421181	−1.168963	−3.017255
57	6	0	−2.595730	−0.731138	−2.310776
58	6	0	−2.579395	0.730995	−2.293984
59	6	0	−1.408529	1.185934	−3.025700
60	6	0	−0.687101	0.009495	−3.462528
61	3	0	−1.403930	−0.112195	−0.470233

$Li^+@C_{60}^-$ dimer (singlet) by M06-2x/6-31G(d) without solvent parameters

E(RM062X) = −4586.03185776 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4585.334138 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.906322	−0.748793	1.173110
2	6	0	7.443136	−2.048946	0.725488
3	6	0	7.443067	−2.048984	−0.728616
4	6	0	7.906194	−0.748846	−1.176340
5	6	0	8.188732	0.055396	−0.001648
6	6	0	5.789761	1.452177	−3.016883
7	6	0	7.032482	1.259317	−2.298895
8	6	0	7.332902	−0.163342	−2.297721
9	6	0	6.285127	−0.849684	−3.026137
10	6	0	5.322206	0.148780	−3.460047
11	6	0	5.837670	−2.092731	2.593010
12	6	0	4.424440	−2.415534	2.601836
13	6	0	4.143415	−3.195689	1.426053
14	6	0	5.386271	−3.392845	0.692458
15	6	0	6.438805	−2.707126	1.420694
16	6	0	3.018104	0.858848	−3.003999
17	6	0	3.965274	−0.137709	−3.451301
18	6	0	3.488801	−1.446414	−3.007936
19	6	0	2.246723	−1.268156	−2.322900
20	6	0	1.962142	0.178483	−2.284811
21	6	0	3.462074	2.111786	−2.588925
22	6	0	2.876395	2.721184	−1.423500
23	6	0	3.931563	3.411538	−0.693590
24	6	0	5.172258	3.216747	−1.419736
25	6	0	4.879839	2.412716	−2.593295
26	6	0	7.333114	−0.163244	2.294508
27	6	0	7.032690	1.259414	2.295630
28	6	0	5.790045	1.452307	3.013730
29	6	0	5.322538	0.148936	3.457002
30	6	0	6.285429	−0.849551	3.023077
31	6	0	6.438674	−2.707198	−1.423701
32	6	0	5.386200	−3.392880	−0.695338
33	6	0	4.143289	−3.195769	−1.428801
34	6	0	4.424197	−2.415658	−2.604637
35	6	0	5.837438	−2.092851	−2.595979
36	6	0	7.904533	1.414325	−0.001670
37	6	0	7.311476	2.027514	−1.175653
38	6	0	6.361149	3.027990	−0.727599
39	6	0	6.361216	3.028017	0.724327
40	6	0	7.311598	2.027569	1.172347
41	6	0	3.931629	3.411563	0.690541
42	6	0	2.876527	2.721261	1.420600
43	6	0	3.462315	2.111908	2.585985
44	6	0	4.880085	2.412831	2.590193
45	6	0	5.172393	3.216809	1.416569
46	6	0	1.974542	−2.008770	1.152638
47	6	0	1.352614	−1.436232	−0.001271
48	6	0	1.974377	−2.008874	−1.155268
49	6	0	2.948418	−3.014319	−0.722772
50	6	0	2.948489	−3.014295	0.720126
51	6	0	3.018391	0.858996	3.001177
52	6	0	1.962367	0.178591	2.282104
53	6	0	2.246956	−1.268045	2.320273
54	6	0	3.489077	−1.446269	3.005178
55	6	0	3.965605	−0.137540	3.448448
56	6	0	1.382351	0.769303	−1.180925
57	6	0	0.785492	−0.025004	−0.001292
58	6	0	1.382447	0.769368	1.178256
59	6	0	1.878894	2.042971	0.725666
60	6	0	1.878838	2.042928	−0.728435
61	3	0	3.479549	−0.922071	−0.001751
62	6	0	−1.974376	2.008724	−1.155566
63	6	0	−2.948436	3.014221	−0.723212
64	6	0	−2.948512	3.014396	0.719685
65	6	0	−1.974565	2.008940	1.152339
66	6	0	−1.352620	1.436246	−0.001485
67	6	0	−3.018382	−0.858553	3.001308
68	6	0	−1.962363	−0.178248	2.282134
69	6	0	−2.246965	1.268391	2.320084
70	6	0	−3.489082	1.446710	3.004969
71	6	0	−3.965601	0.138045	3.448434
72	6	0	−4.424220	2.415270	−2.604983
73	6	0	−5.837459	2.092456	−2.596274
74	6	0	−6.438697	2.706973	−1.424084
75	6	0	−5.386224	3.392768	−0.695826
76	6	0	−4.143312	3.195555	−1.429263
77	6	0	−5.790032	−1.451877	3.013956
78	6	0	−5.322532	−0.148437	3.457036
79	6	0	−6.285430	0.849980	3.022966
80	6	0	−7.333112	0.163559	2.294499
81	6	0	−7.032682	−1.259097	2.295832
82	6	0	−4.880068	−2.412457	2.590557
83	6	0	−5.172375	−3.216608	1.417052

84	6	0	−3.931611	−3.411463	0.691050
85	6	0	−2.876509	−2.721050	1.421005
86	6	0	−3.462300	−2.111528	2.586301
87	6	0	−2.246736	1.267824	−2.323084
88	6	0	−1.962151	−0.178809	−2.284778
89	6	0	−3.018110	−0.859287	−3.003867
90	6	0	−3.965286	0.137198	−3.451314
91	6	0	−3.488820	1.445972	−3.008142
92	6	0	−4.143434	3.195895	1.425590
93	6	0	−5.386290	3.392935	0.691970
94	6	0	−6.438817	2.707317	1.420310
95	6	0	−5.837678	2.093099	2.592715
96	6	0	−4.424449	2.415911	2.601489
97	6	0	−0.785492	0.025019	−0.001294
98	6	0	−1.382442	−0.769184	1.178372
99	6	0	−1.878881	−2.042856	0.725970
100	6	0	−1.878833	−2.043027	−0.728130
101	6	0	−1.382352	−0.769465	−1.180808
102	6	0	−3.931549	−3.411644	−0.693081
103	6	0	−5.172246	−3.216969	−1.419254
104	6	0	−4.879835	−2.413108	−2.592931
105	6	0	−3.462071	−2.112167	−2.588609
106	6	0	−2.876388	−2.721389	−1.423095
107	6	0	−7.906203	0.748647	−1.176433
108	6	0	−8.188734	−0.055423	−0.001622
109	6	0	−7.906327	0.748941	1.173017
110	6	0	−7.443147	2.049030	0.725203
111	6	0	−7.443084	2.048855	−0.728900
112	6	0	−5.789763	−1.452634	−3.016656
113	6	0	−7.032482	−1.259675	−2.298693
114	6	0	−7.332911	0.162983	−2.297730
115	6	0	−6.285142	0.849224	−3.026247
116	6	0	−5.322216	−0.149300	−3.460013
117	6	0	−7.311589	−2.027420	1.172662
118	6	0	−7.904528	−1.414351	−0.001444
119	6	0	−7.311469	−2.027707	−1.175337
120	6	0	−6.361137	−3.028114	−0.727141
121	6	0	−6.361201	−3.027928	0.724786
122	3	0	−3.479505	0.922008	−0.002075

$Li^{+}@C_{60}^{-}$ dimer (triplet) by UM06-2x/6-31G(d) without solvent parameters

E(UM062X) = −4586.00310477 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4585.317353 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−8.367850	0.485274	0.978247
2	6	0	−8.261226	1.196940	−0.284668
3	6	0	−8.178967	0.217032	−1.353034
4	6	0	−8.218237	−1.099060	−0.743934
5	6	0	−8.338853	−0.929481	0.695163
6	6	0	−5.465360	−3.346131	−0.957701
7	6	0	−6.746387	−3.036429	−0.369300
8	6	0	−7.441869	−2.125820	−1.261514
9	6	0	−6.591060	−1.879540	−2.412218
10	6	0	−5.363499	−2.629645	−2.218946
11	6	0	−6.861637	2.899004	0.816806
12	6	0	−5.605490	3.459778	0.403800
13	6	0	−5.483005	3.279039	−1.038963
14	6	0	−6.681080	2.619489	−1.515227
15	6	0	−7.528747	2.372421	−0.363694
16	6	0	−2.971035	−2.236256	−1.781989
17	6	0	−4.150270	−2.090811	−2.620987
18	6	0	−4.112192	−0.775020	−3.231924
19	6	0	−2.916583	−0.107490	−2.751426
20	6	0	−2.208845	−1.021456	−1.866505
21	6	0	−3.072109	−2.925790	−0.567201
22	6	0	−2.412606	−2.398222	0.611579
23	6	0	−3.261630	−2.650325	1.764421
24	6	0	−4.457431	−3.315477	1.287535
25	6	0	−4.335947	−3.482747	−0.152613
26	6	0	−7.725497	0.988604	2.109335
27	6	0	−7.029871	0.076736	3.003352
28	6	0	−5.831970	0.742008	3.479665
29	6	0	−5.790422	2.059869	2.867084
30	6	0	−6.965330	2.211576	2.033325
31	6	0	−7.368021	0.452430	−2.456540
32	6	0	−6.600637	1.679724	−2.540898
33	6	0	−5.318635	1.366796	−3.134356
34	6	0	−5.287242	−0.054218	−3.415906
35	6	0	−6.556226	−0.621265	−2.998011
36	6	0	−7.671971	−1.804379	1.550786
37	6	0	−6.863836	−2.873670	1.011243
38	6	0	−5.690153	−3.017831	1.851776
39	6	0	−5.776751	−2.037514	2.920803
40	6	0	−7.002767	−1.283043	2.729200
41	6	0	−3.343334	−1.713812	2.788968
42	6	0	−2.577363	−0.486253	2.715120
43	6	0	−3.387093	0.582528	3.252755
44	6	0	−4.659840	0.021086	3.665561
45	6	0	−4.632639	−1.402903	3.380481
46	6	0	−3.056453	2.863969	−0.776809
47	6	0	−2.256254	1.795373	−1.312075
48	6	0	−2.942054	1.257726	−2.488153
49	6	0	−4.166091	2.008825	−2.680432
50	6	0	−4.249544	2.987852	−1.611381
51	6	0	−3.348151	1.853490	2.673295
52	6	0	−2.494741	2.102600	1.520809
53	6	0	−3.181670	3.032511	0.627664
54	6	0	−4.466672	3.320819	1.209735
55	6	0	−4.571026	2.601694	2.475012
56	6	0	−1.567491	−0.508975	−0.727040
57	6	0	−1.581598	0.901162	−0.448517
58	6	0	−1.714527	1.067296	1.001317
59	6	0	−1.753144	−0.249374	1.609818
60	6	0	−1.675802	−1.222497	0.539159
61	3	0	−3.827854	0.949963	0.044745
62	6	0	3.152556	3.018434	−0.697975
63	6	0	4.430427	3.317936	−1.286173
64	6	0	4.545682	2.560643	−2.534527
65	6	0	3.326525	1.799029	−2.716593
66	6	0	2.473416	2.063760	−1.571851
67	6	0	3.342222	−1.768177	−2.767924
68	6	0	2.569152	−0.542786	−2.714325
69	6	0	3.374559	0.520783	−3.274306
70	6	0	4.648616	−0.042146	−3.673979
71	6	0	4.629137	−1.459915	−3.362704
72	6	0	5.454956	3.312095	0.974954
73	6	0	6.655903	2.662766	1.465555
74	6	0	7.503275	2.397371	0.320756
75	6	0	6.835799	2.900097	−0.873206
76	6	0	5.578375	3.473903	−0.475094
77	6	0	5.695895	−3.038812	−1.802970
78	6	0	5.778192	−2.078615	−2.889022
79	6	0	6.998386	−1.313316	−2.708110
80	6	0	7.670967	−1.810570	−1.519170
81	6	0	6.868839	−2.873956	−0.962592
82	6	0	4.464804	−3.332612	−1.234081
83	6	0	4.343607	−3.478256	0.207258
84	6	0	3.077107	−2.915976	0.609968
85	6	0	2.411024	−2.415909	−0.581231
86	6	0	3.264537	−2.683387	−1.724960
87	6	0	3.028135	2.870463	0.709439
88	6	0	2.243273	1.795242	1.257908
89	6	0	2.917508	1.292805	2.449570
90	6	0	4.133880	2.054235	2.635730
91	6	0	4.215174	3.017313	1.547223
92	6	0	5.767233	2.014061	−2.910989
93	6	0	6.947873	2.188127	−2.078068
94	6	0	7.712478	0.972874	−2.131437
95	6	0	7.019598	0.040867	−3.007464
96	6	0	5.818463	0.689097	−3.500336
97	6	0	1.708348	1.036260	−1.032009
98	6	0	1.748541	−0.288229	−1.616853
99	6	0	1.670406	−1.244557	−0.527947
100	6	0	1.556335	−0.509589	0.722607
101	6	0	1.577215	0.892988	0.415601
102	6	0	2.970267	−2.209713	1.808121
103	6	0	4.145204	−2.046535	2.649135
104	6	0	4.096918	−0.719955	3.233836
105	6	0	2.895140	−0.067599	2.739472
106	6	0	2.198078	−0.993987	1.871002
107	6	0	8.164069	0.260615	1.348874
108	6	0	8.212833	−1.064578	0.763902
109	6	0	8.333191	−0.917135	−0.678900
110	6	0	8.359512	0.491505	−0.987038
111	6	0	8.241952	1.221223	0.260740
112	6	0	5.265943	0.008770	3.408973
113	6	0	6.540199	−0.558728	3.004445
114	6	0	7.346466	0.511951	2.445095

115	6	0	6.573551	1.735166	2.509747
116	6	0	5.292120	1.426595	3.101339
117	6	0	6.751633	−3.015350	0.420278
118	6	0	7.440657	−2.087228	1.296811
119	6	0	6.584819	−1.825299	2.441570
120	6	0	5.361929	−2.587286	2.260163
121	6	0	5.470169	−3.322123	1.012112
122	3	0	4.581985	1.437913	−0.088675

$Li^+@C_{60}^-$ (doublet) by UM06-2x/6-31G(d)/IEFPCM(oDCB)

E(UM062X) = −2293.02263490 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2292.687395 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.024610	0.418980	3.365990
2	6	0	2.272545	0.036537	2.728675
3	6	0	2.728852	1.168788	1.942665
4	6	0	1.766363	2.245974	2.104202
5	6	0	0.720607	1.787246	2.985810
6	6	0	−0.135838	3.481971	−0.658678
7	6	0	0.081644	3.454736	0.775397
8	6	0	1.462830	3.069141	1.018274
9	6	0	2.095061	2.848664	−0.258088
10	6	0	1.109673	3.096005	−1.296282
11	6	0	1.383758	−2.232864	2.403378
12	6	0	1.365321	−3.050932	1.209860
13	6	0	2.419226	−2.591426	0.329700
14	6	0	3.090201	−1.479718	0.975967
15	6	0	2.450594	−1.258823	2.260951
16	6	0	−0.181333	1.883860	−3.004495
17	6	0	1.086197	2.312836	−2.442253
18	6	0	2.044348	1.231787	−2.598821
19	6	0	1.387570	0.141228	−3.261666
20	6	0	−0.001074	0.530014	−3.496649
21	6	0	−1.377657	2.248229	−2.386151
22	6	0	−2.447119	1.282749	−2.243531
23	6	0	−3.082248	1.497703	−0.958293
24	6	0	−2.405664	2.603726	−0.306685
25	6	0	−1.350537	3.065188	−1.189699
26	6	0	0.005828	−0.513715	3.504713
27	6	0	−1.375053	−0.124210	3.262379
28	6	0	−2.040788	−1.223201	2.614433
29	6	0	−1.081203	−2.302766	2.456682
30	6	0	0.187497	−1.868670	3.016943
31	6	0	3.339465	0.957272	0.714281
32	6	0	3.523818	−0.395495	0.221212
33	6	0	3.305601	−0.369055	−1.215701
34	6	0	2.997729	0.997372	−1.601328
35	6	0	3.024440	1.815738	−0.417467
36	6	0	−0.606923	2.157160	2.752993
37	6	0	−0.924685	3.009150	1.619654
38	6	0	−2.193470	2.573711	1.065600
39	6	0	−2.645283	1.439863	1.849913
40	6	0	−1.667875	1.191966	2.896484
41	6	0	−3.517559	0.412140	−0.203309
42	6	0	−3.339163	−0.942283	−0.696991
43	6	0	−3.030788	−1.806512	0.436192
44	6	0	−2.991564	−0.986634	1.615397
45	6	0	−3.296418	0.383166	1.230398
46	6	0	0.937940	−2.992670	−1.601676
47	6	0	0.621269	−2.146088	−2.745578
48	6	0	1.676198	−1.179718	−2.883052
49	6	0	2.658045	−1.430383	−1.834268
50	6	0	2.211335	−2.563332	−1.049226
51	6	0	−2.092857	−2.842945	0.273637
52	6	0	−1.461783	−3.059732	−0.998414
53	6	0	−0.072037	−3.438732	−0.753674
54	6	0	0.145936	−3.475340	0.678600
55	6	0	−1.099918	−3.090116	1.311425
56	6	0	−1.027394	−0.400385	−3.358914
57	6	0	−0.722888	−1.775577	−2.977849
58	6	0	−1.765356	−2.233005	−2.099488
59	6	0	−2.728820	−1.147749	−1.931156
60	6	0	−2.277801	−0.017514	−2.723136
61	3	0	−0.245577	−0.867290	−0.805645

$Li^+@C_{60}^-$ dimer (singlet) by M06-2x/6-31G(d)/IEFPCM(oDCB)

E(RM062X) = −4586.08059139 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4585.374323 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.886215	−0.791309	1.208274
2	6	0	7.428491	−2.077556	0.715161
3	6	0	7.453789	−2.035002	−0.737269
4	6	0	7.926195	−0.721935	−1.139410
5	6	0	8.189913	0.046528	0.062821
6	6	0	5.846257	1.533964	−2.949735
7	6	0	7.078796	1.320914	−2.218882
8	6	0	7.373784	−0.102669	−2.252585
9	6	0	6.338332	−0.765944	−3.021210
10	6	0	5.384678	0.243864	−3.438008
11	6	0	5.791409	−2.171805	2.553995
12	6	0	4.380421	−2.493779	2.531734
13	6	0	4.118539	−3.239559	1.323662
14	6	0	5.371382	−3.416162	0.608122
15	6	0	6.410416	−2.752244	1.372859
16	6	0	3.072634	0.943307	−3.008031
17	6	0	4.026124	−0.041787	−3.470581
18	6	0	3.542728	−1.361753	−3.071707
19	6	0	2.285622	−1.201390	−2.401740
20	6	0	2.003544	0.242697	−2.323147
21	6	0	3.511562	2.180455	−2.541699
22	6	0	2.908375	2.752675	−1.367475
23	6	0	3.950451	3.424152	−0.601959
24	6	0	5.202521	3.252467	−1.312735
25	6	0	4.930078	2.482639	−2.514299
26	6	0	7.296675	−0.237564	2.337173
27	6	0	6.998378	1.185085	2.375762
28	6	0	5.743491	1.358141	3.078815
29	6	0	5.268656	0.042049	3.476065
30	6	0	6.236230	−0.942739	3.029676
31	6	0	6.459566	−2.669373	−1.466831
32	6	0	5.396358	−3.376620	−0.778645
33	6	0	4.167702	−3.161386	−1.527658
34	6	0	4.469239	−2.342524	−2.679024
35	6	0	5.878817	−2.020263	−2.632577
36	6	0	7.908343	1.406684	0.098133
37	6	0	7.339632	2.056763	−1.068427
38	6	0	6.380112	3.043136	−0.606188
39	6	0	6.354335	3.001270	0.844878
40	6	0	7.294049	1.984501	1.278555
41	6	0	3.925761	3.384203	0.781566
42	6	0	2.858276	2.672490	1.471543
43	6	0	3.423145	2.030669	2.628629
44	6	0	4.841247	2.331693	2.667724
45	6	0	5.153549	3.170751	1.523694
46	6	0	1.975351	−2.028852	1.047780
47	6	0	1.366573	−1.427569	−0.096027
48	6	0	2.010169	−1.963134	−1.250778
49	6	0	2.970924	−2.988996	−0.834922
50	6	0	2.946194	−3.028831	0.603713
51	6	0	2.970890	0.766398	3.000096
52	6	0	1.924037	0.107963	2.246127
53	6	0	2.203959	−1.339748	2.249888
54	6	0	3.441921	−1.535792	2.943261
55	6	0	3.911066	−0.243326	3.431302
56	6	0	1.399515	0.803809	−1.211891
57	6	0	0.786245	−0.023280	−0.062476
58	6	0	1.360205	0.735585	1.152305
59	6	0	1.868845	2.017571	0.743217
60	6	0	1.894369	2.058916	−0.710748
61	3	0	3.505892	−0.436013	−0.180346
62	6	0	−2.010212	1.963014	−1.251013
63	6	0	−2.970952	2.988940	−0.835354
64	6	0	−2.946183	3.029027	0.603280
65	6	0	−1.975323	2.029088	1.047510
66	6	0	−1.366527	1.427658	−0.096197
67	6	0	−2.970919	−0.765895	3.000132
68	6	0	−1.924019	−0.107566	2.246150
69	6	0	−2.203905	1.340150	2.249738
70	6	0	−3.441885	1.536299	2.943102
71	6	0	−3.911041	0.243876	3.431280
72	6	0	−4.469281	2.342132	−2.679329
73	6	0	−5.878847	2.019876	−2.632843
74	6	0	−6.459590	2.669151	−1.467213
75	6	0	−5.396382	3.376559	−0.779177

76	6	0	−4.167715	3.161217	−1.528124
77	6	0	−5.743483	−1.357692	3.079004
78	6	0	−5.268632	−0.041535	3.475993
79	6	0	−6.236245	0.943163	3.029543
80	6	0	−7.296684	0.237868	2.337147
81	6	0	−6.998386	−1.184776	2.375942
82	6	0	−4.841230	−2.331275	2.668023
83	6	0	−5.153514	−3.170533	1.524153
84	6	0	−3.925709	−3.384131	0.782084
85	6	0	−2.858246	−2.672242	1.471926
86	6	0	−3.423129	−2.030245	2.628891
87	6	0	−2.285688	1.201068	−2.401817
88	6	0	−2.003577	−0.242991	−2.323042
89	6	0	−3.072665	−0.943709	−3.007797
90	6	0	−4.026178	0.041296	−3.470520
91	6	0	−3.542775	1.361314	−3.071869
92	6	0	−4.118587	3.239736	1.323120
93	6	0	−5.371431	3.416208	0.607591
94	6	0	−6.410441	2.752406	1.372437
95	6	0	−5.791392	2.172140	2.553636
96	6	0	−4.380437	2.494171	2.531373
97	6	0	−0.786231	0.023324	−0.062459
98	6	0	−1.360169	−0.735380	1.152434
99	6	0	−1.868759	−2.017458	0.743547
100	6	0	−1.894224	−2.059076	−0.710433
101	6	0	−1.399486	−0.803966	−1.211752
102	6	0	−3.950412	−3.424239	−0.601441
103	6	0	−5.202488	−3.252699	−1.312269
104	6	0	−4.930071	−2.483012	−2.513922
105	6	0	−3.511572	−2.180773	−2.541246
106	6	0	−2.908349	−2.752828	−1.366983
107	6	0	−7.926186	0.721738	−1.139496
108	6	0	−8.189934	−0.046565	0.062842
109	6	0	−7.886256	0.791442	1.208182
110	6	0	−7.428549	2.077634	0.714871
111	6	0	−7.453787	2.034851	−0.737549
112	6	0	−5.846268	−1.534423	−2.949567
113	6	0	−7.078796	−1.321272	−2.218709
114	6	0	−7.373786	0.102308	−2.252589
115	6	0	−6.338345	0.765488	−3.021281
116	6	0	−5.384723	−0.244365	−3.438001
117	6	0	−7.294061	−1.984378	1.278852
118	6	0	−7.908313	−1.406705	0.098333
119	6	0	−7.339595	−2.056944	−1.068132
120	6	0	−6.380082	−3.043261	−0.605748
121	6	0	−6.354312	−3.001174	0.845315
122	3	0	−3.506130	0.435051	−0.180507

$Li^{+}@C_{60}^{-}$ dimer (triplet) by UM06-2x/6-31G(d)/IEFPCM(oDCB)

E(UM062X) = − 4586.05582601 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4585.362046 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−8.294980	0.816373	0.992763
2	6	0	−8.187624	1.417520	−0.319506
3	6	0	−8.219321	0.355124	−1.312586
4	6	0	−8.336168	−0.904899	−0.603477
5	6	0	−8.378511	−0.614585	0.820589
6	6	0	−5.767979	−3.372001	−0.745860
7	6	0	−6.992515	−2.913807	−0.133640
8	6	0	−7.661940	−2.024934	−1.068048
9	6	0	−6.840987	−1.932002	−2.261049
10	6	0	−5.666955	−2.765291	−2.056947
11	6	0	−6.605210	3.071954	0.588380
12	6	0	−5.330040	3.515003	0.087681
13	6	0	−5.290827	3.216613	−1.330943
14	6	0	−6.563014	2.622078	−1.719857
15	6	0	−7.369877	2.521860	−0.522819
16	6	0	−3.235544	−2.514532	−1.733478
17	6	0	−4.434227	−2.348186	−2.545500
18	6	0	−4.320986	−1.093489	−3.260389
19	6	0	−3.055305	−0.486037	−2.866346
20	6	0	−2.376371	−1.376224	−1.947274
21	6	0	−3.338321	−3.095804	−0.470765
22	6	0	−2.578793	−2.541207	0.643230
23	6	0	−3.393963	−2.637885	1.835724
24	6	0	−4.658923	−3.240614	1.453274
25	6	0	−4.615855	−3.531020	0.031003
26	6	0	−7.564261	1.352151	2.061166
27	6	0	−6.892449	0.460820	2.989492
28	6	0	−5.628442	1.066351	3.374869
29	6	0	−5.511580	2.323604	2.663742
30	6	0	−6.711077	2.493622	1.852134
31	6	0	−7.441541	0.442397	−2.457749
32	6	0	−6.586791	1.599030	−2.671190
33	6	0	−5.363382	1.141217	−3.289072
34	6	0	−5.447238	−0.294635	−3.457927
35	6	0	−6.736289	−0.730452	−2.945095
36	6	0	−7.737928	−1.469685	1.714942
37	6	0	−7.035112	−2.634179	1.231240
38	6	0	−5.838460	−2.803128	2.040441
39	6	0	−5.808304	−1.746746	3.033920
40	6	0	−6.977862	−0.915027	2.825087
41	6	0	−3.364435	−1.623935	2.789576
42	6	0	−2.511257	−0.469787	2.584419
43	6	0	−3.217369	0.701791	3.070707
44	6	0	−4.506079	0.268479	3.575049
45	6	0	−4.595860	−1.168576	3.402532
46	6	0	−2.899326	2.622848	−1.115979
47	6	0	−2.202516	1.456946	−1.596038
48	6	0	−2.970601	0.896335	−2.706431
49	6	0	−4.139150	1.725851	−2.920293
50	6	0	−4.106009	2.782940	−1.926140
51	6	0	−3.106536	1.908434	2.391128
52	6	0	−2.281465	2.004020	1.200990
53	6	0	−2.948816	2.904103	0.264518
54	6	0	−4.170001	3.357776	0.869519
55	6	0	−4.277796	2.740296	2.182906
56	6	0	−1.647913	−0.833428	−0.870168
57	6	0	−1.561888	0.589036	−0.694727
58	6	0	−1.608242	0.881334	0.736033
59	6	0	−1.727356	−0.380438	1.441295
60	6	0	−1.759818	−1.438596	0.446340
61	3	0	−4.305125	0.804231	−0.570624
62	6	0	2.954749	2.896056	−0.271946
63	6	0	4.173871	3.349879	−0.890375
64	6	0	4.271063	2.712512	−2.197114
65	6	0	3.093443	1.884265	−2.396434
66	6	0	2.285860	1.985412	−1.201452
67	6	0	3.356740	−1.663824	−2.751965
68	6	0	2.504396	−0.502148	−2.558253
69	6	0	3.205898	0.658726	−3.072999
70	6	0	4.487432	0.227229	−3.575273
71	6	0	4.586606	−1.210343	−3.378517
72	6	0	5.292812	3.261001	1.311265
73	6	0	6.559700	2.658243	1.692053
74	6	0	7.369960	2.549022	0.491146
75	6	0	6.607721	3.093242	−0.621442
76	6	0	5.336050	3.533642	−0.117154
77	6	0	5.832567	−2.827803	−2.005262
78	6	0	5.797153	−1.779895	−3.005848
79	6	0	6.975218	−0.944125	−2.812897
80	6	0	7.736831	−1.481912	−1.708042
81	6	0	7.030587	−2.636279	−1.201604
82	6	0	4.656463	−3.263817	−1.409592
83	6	0	4.615186	−3.528778	0.017613
84	6	0	3.333254	−3.095162	0.519068
85	6	0	2.574882	−2.557943	−0.592153
86	6	0	3.390568	−2.664201	−1.791613
87	6	0	2.910018	2.631946	1.104208
88	6	0	2.203360	1.484254	1.606365
89	6	0	2.969215	0.942527	2.712112
90	6	0	4.147596	1.775855	2.905562
91	6	0	4.114663	2.825601	1.909561
92	6	0	5.507940	2.290304	−2.680623
93	6	0	6.707368	2.491176	−1.884959
94	6	0	7.554139	1.339150	−2.077083
95	6	0	6.879471	0.431013	−2.998937
96	6	0	5.622899	1.027314	−3.391238
97	6	0	1.615090	0.866284	−0.708274
98	6	0	1.724210	−0.406016	−1.411565
99	6	0	1.757352	−1.451179	−0.409910
100	6	0	1.659901	−0.819625	0.900648
101	6	0	1.557944	0.606532	0.711695
102	6	0	3.238107	−2.489903	1.775330
103	6	0	4.436601	−2.299186	2.575002
104	6	0	4.322721	−1.031671	3.276234
105	6	0	3.064482	−0.432873	2.891741
106	6	0	2.387719	−1.341617	1.969775
107	6	0	8.217383	0.392463	1.303692

108	6	0	8.332249	−0.877101	0.605479
109	6	0	8.378878	−0.610846	−0.818352
110	6	0	8.282247	0.814414	−1.008083
111	6	0	8.181590	1.441104	0.303895
112	6	0	5.452670	−0.233374	3.463467
113	6	0	6.735140	−0.670838	2.954513
114	6	0	7.440812	0.491791	2.450567
115	6	0	6.590037	1.651957	2.648375
116	6	0	5.359723	1.200202	3.275551
117	6	0	6.988116	−2.893420	0.165441
118	6	0	7.657419	−1.990084	1.091117
119	6	0	6.844092	−1.886075	2.283450
120	6	0	5.668903	−2.716681	2.090695
121	6	0	5.765720	−3.347549	0.785675
122	3	0	4.418190	0.882885	−0.418833

$Li^+@C_{60}^-$ (doublet) by UM06-2x/6-31G(d)/SMD(oDCB)

E(UM062X) = −2293.06177226 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2292.727184 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.024609	0.424407	3.371503
2	6	0	2.272445	0.042068	2.732036
3	6	0	2.727858	1.173743	1.944365
4	6	0	1.767710	2.251482	2.108392
5	6	0	0.719774	1.789060	2.987751
6	6	0	−0.135524	3.485451	−0.653576
7	6	0	0.081667	3.458915	0.779069
8	6	0	1.461988	3.069297	1.021404
9	6	0	2.096987	2.852743	−0.256371
10	6	0	1.108544	3.098603	−1.293391
11	6	0	1.380803	−2.224874	2.401400
12	6	0	1.364813	−3.046971	1.210816
13	6	0	2.412362	−2.584253	0.329782
14	6	0	3.086151	−1.472189	0.975310
15	6	0	2.448074	−1.250896	2.261202
16	6	0	−0.182571	1.882777	−2.994148
17	6	0	1.086194	2.313819	−2.437487
18	6	0	2.051390	1.240388	−2.606013
19	6	0	1.383089	0.142478	−3.247746
20	6	0	−0.004490	0.533282	−3.484187
21	6	0	−1.378324	2.252477	−2.379944
22	6	0	−2.443833	1.285470	−2.237332
23	6	0	−3.078441	1.500014	−0.951488
24	6	0	−2.403699	2.607936	−0.300309
25	6	0	−1.352641	3.072508	−1.185504
26	6	0	0.005069	−0.508945	3.506525
27	6	0	−1.376120	−0.119616	3.262889
28	6	0	−2.049628	−1.223087	2.623373
29	6	0	−1.083249	−2.291513	2.453338
30	6	0	0.185993	−1.857720	3.012650
31	6	0	3.339405	0.962652	0.717485
32	6	0	3.519405	−0.389661	0.222238
33	6	0	3.296223	−0.361931	−1.213696
34	6	0	3.002552	1.001179	−1.603638
35	6	0	3.017749	1.816053	−0.414760
36	6	0	−0.605923	2.162636	2.756211
37	6	0	−0.924962	3.015379	1.626126
38	6	0	−2.195437	2.579721	1.072188
39	6	0	−2.650810	1.446699	1.855954
40	6	0	−1.666182	1.193533	2.895950
41	6	0	−3.514151	0.415991	−0.199363
42	6	0	−3.332763	−0.936334	−0.694716
43	6	0	−3.026564	−1.797839	0.436822
44	6	0	−2.997267	−0.982728	1.620333
45	6	0	−3.295596	0.386923	1.234494
46	6	0	0.937491	−2.997676	−1.609507
47	6	0	0.620306	−2.155668	−2.756795
48	6	0	1.671728	−1.178412	−2.879665
49	6	0	2.658222	−1.429733	−1.834965
50	6	0	2.209773	−2.560302	−1.051768
51	6	0	−2.094465	−2.836175	0.272757
52	6	0	−1.466463	−3.059183	−1.001431
53	6	0	−0.074243	−3.441645	−0.754467
54	6	0	0.141747	−3.470893	0.677520
55	6	0	−1.102503	−3.081013	1.310400
56	6	0	−1.028386	−0.399092	−3.353183
57	6	0	−0.729460	−1.779489	−2.988932
58	6	0	−1.769595	−2.232740	−2.104190
59	6	0	−2.730065	−1.143699	−1.930102
60	6	0	−2.276276	−0.013962	−2.715943
61	3	0	−0.172664	−1.093425	−0.922025

$Li^+@C_{60}^-$ dimer (singlet) by M06-2x/6-31G(d)/SMD(oDCB)

E(RM062X) = −4586.15317113 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4585.451554 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−7.909469	−0.752309	−1.174588
2	6	0	−7.444521	−2.051352	−0.726110
3	6	0	−7.444562	−2.050901	0.727336
4	6	0	−7.909539	−0.751517	1.174937
5	6	0	−8.192938	0.051948	−0.000092
6	6	0	−5.794143	1.451276	3.013474
7	6	0	−7.036651	1.257202	2.296203
8	6	0	−7.336975	−0.165297	2.296446
9	6	0	−6.288694	−0.850425	3.025332
10	6	0	−5.326561	0.148692	3.458939
11	6	0	−5.840185	−2.094866	−2.593365
12	6	0	−4.426989	−2.417280	−2.602826
13	6	0	−4.145921	−3.196252	−1.425988
14	6	0	−5.388404	−3.395683	−0.692902
15	6	0	−6.440705	−2.709615	−1.421324
16	6	0	−3.023985	0.860254	3.001484
17	6	0	−3.969590	−0.137082	3.450659
18	6	0	−3.492329	−1.445461	3.007761
19	6	0	−2.250147	−1.265863	2.323815
20	6	0	−1.967012	0.181054	2.283842
21	6	0	−3.467391	2.113802	2.587610
22	6	0	−2.882388	2.723614	1.422150
23	6	0	−3.938623	3.411865	0.691102
24	6	0	−5.178785	3.216510	1.417332
25	6	0	−4.885270	2.413767	2.591642
26	6	0	−7.336885	−0.166836	−2.296484
27	6	0	−7.036538	1.255680	−2.297131
28	6	0	−5.794018	1.449274	−3.014476
29	6	0	−5.326428	0.146397	−3.459091
30	6	0	−6.288562	−0.852434	−3.024796
31	6	0	−6.440753	−2.708636	1.423017
32	6	0	−5.388423	−3.395166	0.695103
33	6	0	−4.145969	−3.195353	1.428138
34	6	0	−4.427083	−2.415542	2.604455
35	6	0	−5.840226	−2.093099	2.594691
36	6	0	−7.911322	1.411693	−0.000538
37	6	0	−7.316985	2.025108	1.173032
38	6	0	−6.367474	3.025671	0.724706
39	6	0	−6.367481	3.025270	−0.726814
40	6	0	−7.316902	2.024327	−1.174495
41	6	0	−3.938592	3.411418	−0.693352
42	6	0	−2.882340	2.722652	−1.423864
43	6	0	−3.467296	2.112050	−2.588966
44	6	0	−4.885170	2.412080	−2.593281
45	6	0	−5.178723	3.215610	−1.419498
46	6	0	−1.981559	−2.005283	−1.152596
47	6	0	−1.361792	−1.430613	0.000522
48	6	0	−1.981772	−2.004301	1.153933
49	6	0	−2.951531	−3.013971	0.722460
50	6	0	−2.951355	−3.014699	−0.720476
51	6	0	−3.023887	0.858188	−3.001879
52	6	0	−1.966944	0.179481	−2.283727
53	6	0	−2.250025	−1.267486	−2.322859
54	6	0	−3.492198	−1.447498	−3.006761
55	6	0	−3.969471	−0.139385	−3.450420
56	6	0	−1.387051	0.771600	1.179565
57	6	0	−0.787797	−0.022497	0.000098
58	6	0	−1.387012	0.770819	−1.179901
59	6	0	−1.886559	2.043321	−0.727698
60	6	0	−1.886612	2.043723	0.726474
61	3	0	−3.535364	−0.934634	−0.000062
62	6	0	1.981500	2.004731	1.153182
63	6	0	2.951284	3.014262	0.721269
64	6	0	2.951164	3.014314	−0.721664
65	6	0	1.981538	2.004615	−1.153328
66	6	0	1.361631	1.430483	0.000023
67	6	0	3.023924	−0.859538	−3.001569
68	6	0	1.966943	−0.180603	−2.283665
69	6	0	2.249979	1.266366	−2.323261

70	6	0	3.492086	1.446209	−3.007291
71	6	0	3.969422	0.137964	−3.450529
72	6	0	4.426937	2.416570	2.603482
73	6	0	5.840099	2.094242	2.593845
74	6	0	6.440561	2.709341	1.421926
75	6	0	5.388176	3.395523	0.693734
76	6	0	4.145727	3.195911	1.426852
77	6	0	5.794121	−1.450384	−3.013944
78	6	0	5.326404	−0.147722	−3.459009
79	6	0	6.288495	0.851355	−3.025190
80	6	0	7.336871	0.166118	−2.296565
81	6	0	7.036642	−1.256416	−2.296679
82	6	0	4.885326	−2.413028	−2.592283
83	6	0	5.178953	−3.216066	−1.418213
84	6	0	3.938850	−3.411742	−0.691976
85	6	0	2.882520	−2.723349	−1.422767
86	6	0	3.467424	−2.113173	−2.588119
87	6	0	2.250059	1.266662	2.323307
88	6	0	1.967117	−0.180296	2.283825
89	6	0	3.024119	−0.859132	3.001751
90	6	0	3.969640	0.138427	3.450534
91	6	0	3.492252	1.446605	3.007194
92	6	0	4.145694	3.195701	−1.427263
93	6	0	5.388138	3.395423	−0.694261
94	6	0	6.440483	2.709135	−1.422412
95	6	0	5.839975	2.093884	−2.594184
96	6	0	4.426767	2.416237	−2.603781
97	6	0	0.787814	0.022235	0.000110
98	6	0	1.387077	−0.771511	−1.179574
99	6	0	1.886700	−2.043805	−0.726872
100	6	0	1.886728	−2.043724	0.727311
101	6	0	1.387124	−0.771393	1.179856
102	6	0	3.938876	−3.411669	0.692477
103	6	0	5.179040	−3.215972	1.418619
104	6	0	4.885488	−2.412776	2.592622
105	6	0	3.467572	−2.112857	2.588446
106	6	0	2.882606	−2.723203	1.423250
107	6	0	7.909466	0.752214	1.174601
108	6	0	8.192944	−0.051688	−0.000108
109	6	0	7.909434	0.752088	−1.174922
110	6	0	7.444418	2.051320	−0.726960
111	6	0	7.444362	2.051342	0.726487
112	6	0	5.794280	−1.450011	3.014017
113	6	0	7.036742	−1.256116	2.296654
114	6	0	7.336967	0.166413	2.296368
115	6	0	6.288646	0.851740	3.024945
116	6	0	5.326622	−0.147263	3.459008
117	6	0	7.317079	−2.024598	−1.173728
118	6	0	7.911436	−1.411455	−0.000011
119	6	0	7.317134	−2.024457	1.173804
120	6	0	6.367745	−3.025341	0.725915
121	6	0	6.367672	−3.025340	−0.725607
122	3	0	3.534804	0.933751	0.000789

$Li^{+}@C_{60}^{-}$ dimer (triplet) by UM06-2x/6-31G(d)/SMD(oDCB)

E(UM062X) = −4586.12808508 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4585.439240 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−8.418104	0.831361	−0.435001
2	6	0	−8.312565	−0.437635	−1.136392
3	6	0	−8.206655	−1.494801	−0.147371
4	6	0	−8.233298	−0.872623	1.162738
5	6	0	−8.369731	0.563456	0.981166
6	6	0	−5.451310	−1.041768	3.376276
7	6	0	−6.740425	−0.466742	3.077844
8	6	0	−7.439830	−1.374035	2.184689
9	6	0	−6.583615	−2.520311	1.939107
10	6	0	−5.348159	−2.308759	2.670736
11	6	0	−6.944408	0.658198	−2.868932
12	6	0	−5.691739	0.249485	−3.440479
13	6	0	−5.555060	−1.189136	−3.246993
14	6	0	−6.739846	−1.667880	−2.565984
15	6	0	−7.594857	−0.521940	−2.320773
16	6	0	−2.966304	−1.855368	2.240859
17	6	0	−4.138855	−2.705419	2.119202
18	6	0	−4.111795	−3.331804	0.809668
19	6	0	−2.929673	−2.848343	0.121833
20	6	0	−2.220593	−1.944684	1.016551
21	6	0	−3.066355	−0.634923	2.921883
22	6	0	−2.423081	0.543915	2.373632
23	6	0	−3.278234	1.691762	2.623448
24	6	0	−4.461417	1.212221	3.308711
25	6	0	−4.326391	−0.224971	3.488842
26	6	0	−7.791004	1.962531	−0.958535
27	6	0	−7.091291	2.872087	−0.064723
28	6	0	−5.907004	3.352899	−0.750440
29	6	0	−5.877056	2.724618	−2.060931
30	6	0	−7.046321	1.879796	−2.189245
31	6	0	−7.389560	−2.594108	−0.382624
32	6	0	−6.637734	−2.683582	−1.618882
33	6	0	−5.346902	−3.263483	−1.316494
34	6	0	−5.294976	−3.530736	0.106123
35	6	0	−6.559571	−3.117934	0.685233
36	6	0	−7.698825	1.434688	1.839994
37	6	0	−6.871478	0.911995	2.901792
38	6	0	−5.702278	1.762771	3.020337
39	6	0	−5.811429	2.823396	2.033744
40	6	0	−7.045739	2.613191	1.297773
41	6	0	−3.381100	2.707014	1.679427
42	6	0	−2.630966	2.626198	0.442508
43	6	0	−3.458630	3.147199	−0.620925
44	6	0	−4.726151	3.554896	−0.047095
45	6	0	−4.678949	3.284355	1.378889
46	6	0	−3.127959	−0.902124	−2.863348
47	6	0	−2.308701	−1.420131	−1.800453
48	6	0	−2.975267	−2.597224	−1.245012
49	6	0	−4.207422	−2.808178	−1.978826
50	6	0	−4.313819	−1.748980	−2.965966
51	6	0	−3.431958	2.554413	−1.885930
52	6	0	−2.574501	1.406358	−2.132797
53	6	0	−3.266812	0.497637	−3.043632
54	6	0	−4.558040	1.067434	−3.324672
55	6	0	−4.662773	2.338208	−2.616151
56	6	0	−1.593686	−0.806248	0.486764
57	6	0	−1.628152	−0.541742	−0.925752
58	6	0	−1.777559	0.903133	−1.103728
59	6	0	−1.802738	1.525460	0.206945
60	6	0	−1.701841	0.465797	1.189595
61	3	0	−3.947942	−0.080641	−0.938687
62	6	0	3.352332	−0.556767	−3.126445
63	6	0	4.665921	−1.090739	−3.374555
64	6	0	4.792349	−2.358566	−2.656370
65	6	0	3.548193	−2.601828	−1.956798
66	6	0	2.665475	−1.479117	−2.229968
67	6	0	3.408456	−2.749052	1.602572
68	6	0	2.689761	−2.687661	0.346857
69	6	0	3.559292	−3.190615	−0.693509
70	6	0	4.821848	−3.562620	−0.084464
71	6	0	4.728329	−3.289753	1.338291
72	6	0	5.603540	1.200564	−3.269098
73	6	0	6.755489	1.713911	−2.559470
74	6	0	7.631033	0.591739	−2.286206
75	6	0	7.033056	−0.610672	−2.848489
76	6	0	5.785171	−0.239776	−3.457114
77	6	0	5.667017	−1.737636	3.002891
78	6	0	5.830952	−2.795550	2.021072
79	6	0	7.077314	−2.553580	1.318527
80	6	0	7.683024	−1.354631	1.876430
81	6	0	6.814579	−0.855155	2.915652
82	6	0	4.403591	−1.222057	3.258655
83	6	0	4.225478	0.211276	3.435380
84	6	0	2.971473	0.585496	2.828143
85	6	0	2.373861	−0.613963	2.265907
86	6	0	3.253390	−1.734574	2.542004
87	6	0	3.172245	0.842238	−2.951755
88	6	0	2.320931	1.333649	−1.898564
89	6	0	2.928693	2.534981	−1.335547
90	6	0	4.171085	2.781021	−2.034711
91	6	0	4.332566	1.721016	−3.020170
92	6	0	6.002888	−2.708982	−2.069050
93	6	0	7.156647	−1.831741	−2.167009
94	6	0	7.867040	−1.889212	−0.918407
95	6	0	7.168103	−2.814286	−0.041137
96	6	0	6.015535	−3.331286	−0.756554
97	6	0	1.834005	−0.996365	−1.224062
98	6	0	1.839571	−1.613344	0.084265
99	6	0	1.684306	−0.554059	1.064071
100	6	0	1.557944	0.710951	0.358358
101	6	0	1.647813	0.443389	−1.049336

102	6	0	2.853014	1.799333	2.148326
103	6	0	4.002213	2.684520	2.060542
104	6	0	3.990958	3.304530	0.747762
105	6	0	2.837904	2.786238	0.029560
106	6	0	2.134402	1.868409	0.901340
107	6	0	8.162888	1.585214	−0.098554
108	6	0	8.172425	0.966588	1.211174
109	6	0	8.350905	−0.467110	1.033610
110	6	0	8.448501	−0.736071	−0.379809
111	6	0	8.320265	0.527391	−1.082132
112	6	0	5.183822	3.536377	0.076687
113	6	0	6.445857	3.161588	0.689360
114	6	0	7.317018	2.659535	−0.358135
115	6	0	6.597145	2.730308	−1.611141
116	6	0	5.282808	3.269083	−1.346108
117	6	0	6.642531	0.520543	3.087718
118	6	0	7.337660	1.444441	2.212524
119	6	0	6.454457	2.566202	1.942252
120	6	0	5.207337	2.323486	2.644862
121	6	0	5.328742	1.059257	3.351215
122	3	0	4.590091	0.080233	−1.359988

$Li^+@C_{60}^-$ (doublet) by UωB97XD/6-31G(d) without solvent parameters

E(UwB97XD) = −2293.00616263 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2292.673113 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.427563	1.176631	3.015438
2	6	0	0.699018	0.000666	3.450675
3	6	0	1.428266	−1.175180	3.014886
4	6	0	2.594453	−0.725377	2.290022
5	6	0	2.593748	0.727874	2.290262
6	6	0	3.030339	−1.416555	−1.170802
7	6	0	3.480230	−0.695428	−0.001806
8	6	0	3.030032	−1.416692	1.167525
9	6	0	2.305622	−2.593678	0.723394
10	6	0	2.305425	−2.593374	−0.726414
11	6	0	−1.414731	1.177190	3.013805
12	6	0	−2.574392	0.732147	2.291607
13	6	0	−2.573200	−0.732671	2.290632
14	6	0	−1.413429	−1.177625	3.013779
15	6	0	−0.687983	0.000011	3.450613
16	6	0	0.732667	−2.303428	−2.594052
17	6	0	1.188081	−3.026708	−1.421185
18	6	0	0.017422	−3.477465	−0.693819
19	6	0	−1.154234	−3.025998	−1.423724
20	6	0	−0.709508	−2.312943	−2.596733
21	6	0	1.428717	−1.174726	−3.018541
22	6	0	0.699486	0.001070	−3.453739
23	6	0	1.427852	1.177170	−3.018821
24	6	0	2.593924	0.728067	−2.293409
25	6	0	2.594521	−0.725279	−2.293557
26	6	0	0.730895	2.304748	2.590876
27	6	0	1.185626	3.028399	1.418154
28	6	0	0.014794	3.478584	0.690819
29	6	0	−1.156674	3.026530	1.420376
30	6	0	−0.711516	2.312933	2.593182
31	6	0	0.733228	−2.303874	2.590985
32	6	0	−0.709866	−2.313181	2.593156
33	6	0	−1.154325	−3.027083	1.421250
34	6	0	0.017468	−3.477678	0.691290
35	6	0	1.188436	−3.027314	1.418460
36	6	0	3.028788	1.419459	1.167535
37	6	0	3.479426	0.698569	−0.001571
38	6	0	3.028765	1.419479	−1.170725
39	6	0	2.303410	2.596153	−0.726421
40	6	0	2.303366	2.595896	0.723282
41	6	0	0.731357	2.305444	−2.594287
42	6	0	−0.711012	2.313926	−2.596798
43	6	0	−1.156436	3.027489	−1.424200
44	6	0	0.014882	3.479019	−0.694283
45	6	0	1.185995	3.028965	−1.421430
46	6	0	−3.501594	−0.715045	−0.002551
47	6	0	−3.018186	−1.424859	−1.165310
48	6	0	−2.280591	−2.603072	−0.723261
49	6	0	−2.280439	−2.603218	0.720288
50	6	0	−3.016004	−1.424793	1.161427
51	6	0	−2.281890	2.603170	−0.723771
52	6	0	−3.016329	1.423793	−1.165072
53	6	0	−3.499897	0.713490	−0.001946
54	6	0	−3.015791	1.422934	1.160731
55	6	0	−2.281575	2.602211	0.719652
56	6	0	−1.413857	−1.176945	−3.017584
57	6	0	−2.574567	−0.732671	−2.296423
58	6	0	−2.574620	0.732671	−2.296066
59	6	0	−1.414179	1.178065	−3.018087
60	6	0	−0.687830	0.000756	−3.454036
61	3	0	−1.319956	−0.039744	−0.046556

$Li^+@C_{60}^-$ dimer (singlet) by ωB97XD/6-31G(d) without solvent parameters

E(RwB97XD) = −4586.06579217 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4585.367721 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.904608	−0.751849	1.170102
2	6	0	7.439982	−2.050239	0.723104
3	6	0	7.438420	−2.050183	−0.728738
4	6	0	7.902352	−0.751857	−1.176639
5	6	0	8.186075	0.050905	−0.003501
6	6	0	5.788384	1.446485	−3.012659
7	6	0	7.030950	1.254201	−2.296845
8	6	0	7.330174	−0.166238	−2.296088
9	6	0	6.282073	−0.851437	−3.023926
10	6	0	5.320788	0.144394	−3.454860
11	6	0	5.837795	−2.091857	2.589037
12	6	0	4.426460	−2.413237	2.599033
13	6	0	4.144568	−3.192953	1.423500
14	6	0	5.383934	−3.390610	0.692085
15	6	0	6.436387	−2.706624	1.417455
16	6	0	3.019561	0.852359	−2.995337
17	6	0	3.964622	−0.142422	−3.444891
18	6	0	3.489016	−1.447178	−3.001340
19	6	0	2.242203	−1.272442	−2.319416
20	6	0	1.964761	0.172493	−2.275893
21	6	0	3.463387	2.104010	−2.581788
22	6	0	2.879835	2.713489	−1.417820
23	6	0	3.935149	3.403830	−0.690891
24	6	0	5.173045	3.209650	−1.417177
25	6	0	4.880255	2.405531	−2.588445
26	6	0	7.334034	−0.166196	2.290384
27	6	0	7.034700	1.254125	2.291774
28	6	0	5.793535	1.446493	3.009992
29	6	0	5.326707	0.144504	3.453240
30	6	0	6.287256	−0.851495	3.020067
31	6	0	6.433207	−2.706500	−1.420989
32	6	0	5.382453	−3.390676	−0.693597
33	6	0	4.141193	−3.192763	−1.422597
34	6	0	4.421555	−2.413365	−2.599807
35	6	0	5.832514	−2.091628	−2.591507
36	6	0	7.903883	1.409033	−0.003200
37	6	0	7.310509	2.021709	−1.175043
38	6	0	6.361878	3.021447	−0.726616
39	6	0	6.363210	3.021477	0.723007
40	6	0	7.312626	2.021771	1.169629
41	6	0	3.936315	3.403478	0.691759
42	6	0	2.882161	2.713512	1.420883
43	6	0	3.467830	2.104422	2.583807
44	6	0	4.884771	2.405713	2.587754
45	6	0	5.175574	3.209432	1.415757
46	6	0	1.986999	−2.003508	1.151946
47	6	0	1.350903	−1.439910	0.001542
48	6	0	1.978656	−2.006867	−1.149404
49	6	0	2.952699	−3.009490	−0.718186
50	6	0	2.955379	−3.007900	0.720537
51	6	0	3.024712	0.852562	2.997207
52	6	0	1.969621	0.173356	2.279164
53	6	0	2.249724	−1.270937	2.319838
54	6	0	3.495125	−1.446933	3.002109
55	6	0	3.970840	−0.142358	3.445039
56	6	0	1.384526	0.765667	−1.174302
57	6	0	0.782596	−0.027116	0.003347
58	6	0	1.385975	0.765978	1.180208
59	6	0	1.884723	2.036019	0.728528
60	6	0	1.884260	2.035754	−0.723221
61	3	0	3.423501	−0.590173	−0.081076
62	6	0	−1.978776	2.006676	−1.149573

63	6	0	−2.952789	3.009368	−0.718434
64	6	0	−2.955329	3.008028	0.720292
65	6	0	−1.986910	2.003714	1.151781
66	6	0	−1.350916	1.439921	0.001414
67	6	0	−3.024410	−0.852032	2.997655
68	6	0	−1.969396	−0.172946	2.279388
69	6	0	−2.249508	1.271353	2.319829
70	6	0	−3.494839	1.447462	3.002194
71	6	0	−3.970501	0.142962	3.445403
72	6	0	−4.421831	2.412895	−2.599801
73	6	0	−5.832789	2.091150	−2.591301
74	6	0	−6.433369	2.706226	−1.420832
75	6	0	−5.382547	3.390536	−0.693667
76	6	0	−4.141358	3.192502	−1.422757
77	6	0	−5.793228	−1.445977	3.010821
78	6	0	−5.326365	−0.143908	3.453792
79	6	0	−6.286963	0.852010	3.020535
80	6	0	−7.333809	0.166575	2.291077
81	6	0	−7.034466	−1.253744	2.292692
82	6	0	−4.884498	−2.405265	2.588662
83	6	0	−5.175412	−3.209193	1.416837
84	6	0	−3.936224	−3.403359	0.692749
85	6	0	−2.882002	−2.713260	1.421647
86	6	0	−3.467559	−2.103968	2.584521
87	6	0	−2.242439	1.272037	−2.319429
88	6	0	−1.964987	−0.172890	−2.275672
89	6	0	−3.019854	−0.852889	−2.994891
90	6	0	−3.964965	0.141805	−3.444529
91	6	0	−3.489323	1.446644	−3.001258
92	6	0	−4.144451	3.193200	1.423342
93	6	0	−5.383890	3.390720	0.692016
94	6	0	−6.436266	2.706853	1.417612
95	6	0	−5.837553	2.092298	2.589243
96	6	0	−4.426218	2.413690	2.599039
97	6	0	−0.782602	0.027130	0.003419
98	6	0	−1.385857	−0.765756	1.180480
99	6	0	−1.884638	−2.035882	0.729074
100	6	0	−1.884323	−2.035875	−0.722675
101	6	0	−1.384645	−0.765864	−1.174028
102	6	0	−3.935197	−3.403960	−0.689902
103	6	0	−5.173166	−3.209917	−1.416097
104	6	0	−4.880499	−2.406003	−2.587537
105	6	0	−3.463633	−2.104470	−2.581075
106	6	0	−2.879962	−2.713739	−1.417057
107	6	0	−7.902476	0.751615	−1.175992
108	6	0	−8.186077	−0.050939	−0.002683
109	6	0	−7.904498	0.752026	1.170749
110	6	0	−7.439925	2.050339	0.723475
111	6	0	−7.438509	2.050024	−0.728366
112	6	0	−5.788675	−1.447037	−3.011831
113	6	0	−7.031170	−1.254635	−2.295928
114	6	0	−7.330404	0.165803	−2.295394
115	6	0	−6.282380	0.850880	−3.023457
116	6	0	−5.321130	−0.145021	−3.454309
117	6	0	−7.312498	−2.021592	1.170712
118	6	0	−7.903875	−1.409065	−0.002168
119	6	0	−7.310613	−2.021943	−1.173961
120	6	0	−6.361932	−3.021596	−0.725451
121	6	0	−6.363119	−3.021370	0.724173
122	3	0	−3.423515	0.590315	−0.081033

$Li^{+}@C_{60}^{-}$ dimer (triplet) by UωB97XD/6-31G(d) without solvent parameters

E(UwB97XD) = −4586.02920245 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4585.343276 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−8.297314	0.033566	0.266757
2	6	0	−8.298379	−0.651497	−1.005990
3	6	0	−8.082460	−2.061532	−0.745429
4	6	0	−7.973606	−2.251149	0.688398
5	6	0	−8.097534	−0.955524	1.312450
6	6	0	−4.963172	−3.448202	2.177836
7	6	0	−6.275135	−2.858488	2.358936
8	6	0	−7.077638	−3.190525	1.195723
9	6	0	−6.272197	−3.985318	0.304456
10	6	0	−4.964500	−4.136286	0.898658
11	6	0	−7.115564	1.259256	−1.999944
12	6	0	−5.927732	1.281568	−2.832041
13	6	0	−5.804100	−0.021182	−3.460772
14	6	0	−6.912335	−0.837532	−3.027191
15	6	0	−7.718006	−0.054936	−2.121777
16	6	0	−2.641659	−3.415949	0.549299
17	6	0	−3.820170	−4.122159	0.106719
18	6	0	−3.931722	−3.942415	−1.338528
19	6	0	−2.814540	−3.151085	−1.792252
20	6	0	−2.036289	−2.797437	−0.620868
21	6	0	−2.641022	−2.748656	1.772797
22	6	0	−2.035643	−1.445310	1.892763
23	6	0	−2.846409	−0.651435	2.786205
24	6	0	−3.958507	−1.469565	3.230991
25	6	0	−3.831649	−2.770893	2.602194
26	6	0	−7.719587	1.290328	0.383844
27	6	0	−6.917529	1.619507	1.541301
28	6	0	−5.810419	2.436971	1.099613
29	6	0	−5.929851	2.622923	−0.335117
30	6	0	−7.113845	1.913667	−0.778927
31	6	0	−7.305914	−2.819029	−1.610249
32	6	0	−6.706963	−2.200064	−2.776954
33	6	0	−5.404475	−2.785054	−2.959440
34	6	0	−5.203520	−3.785470	−1.907181
35	6	0	−6.379209	−3.804017	−1.082635
36	6	0	−7.328741	−0.636773	2.425402
37	6	0	−6.395871	−1.614295	2.955846
38	6	0	−5.212304	−0.905028	3.401311
39	6	0	−5.418390	0.507913	3.140856
40	6	0	−6.726354	0.670804	2.544235
41	6	0	−3.045496	0.702217	2.535369
42	6	0	−2.444447	1.319080	1.367883
43	6	0	−3.370459	2.303353	0.841720
44	6	0	−4.553385	2.279275	1.669666
45	6	0	−4.353766	1.290336	2.715965
46	6	0	−3.363823	0.122460	−3.198910
47	6	0	−2.428647	−0.863946	−2.672839
48	6	0	−3.009192	−2.177957	−2.817910
49	6	0	−4.329310	−2.001620	−3.386493
50	6	0	−4.542781	−0.582598	−3.642895
51	6	0	−3.483432	2.481426	−0.535309
52	6	0	−2.675259	1.700276	−1.438841
53	6	0	−3.481990	1.367440	−2.589489
54	6	0	−4.795987	1.957823	−2.407506
55	6	0	−4.795723	2.646461	−1.131010
56	6	0	−1.464622	−1.533254	−0.499758
57	6	0	−1.659291	−0.538693	−1.553460
58	6	0	−1.784087	0.748709	−0.930855
59	6	0	−1.672938	0.559028	0.503432
60	6	0	−1.461771	−0.849786	0.765940
61	3	0	−4.277814	−1.580779	−0.977300
62	6	0	2.608194	2.086719	−2.294491
63	6	0	3.836708	1.917060	−3.047054
64	6	0	4.036437	0.496706	−3.302442
65	6	0	2.949232	−0.215186	−2.673869
66	6	0	2.082340	0.768898	−2.038509
67	6	0	3.501187	−2.508153	−0.007779
68	6	0	2.554193	−1.762204	−0.799002
69	6	0	3.177901	−1.443681	−2.061330
70	6	0	4.515436	−2.009655	−2.063540
71	6	0	4.715551	−2.666872	−0.786420
72	6	0	4.882511	3.748738	−1.750158
73	6	0	6.165112	3.804427	−1.108519
74	6	0	7.024108	2.822527	−1.746113
75	6	0	6.273435	2.166346	−2.797830
76	6	0	4.946326	2.726117	−2.797115
77	6	0	6.042967	−2.388923	1.265190
78	6	0	5.953376	−2.606643	−0.166761
79	6	0	7.046106	−1.890897	−0.795920
80	6	0	7.803879	−1.230556	0.251746
81	6	0	7.186476	−1.543924	1.521915
82	6	0	4.879541	−2.237213	2.010080
83	6	0	4.816652	−1.227146	3.052954
84	6	0	3.485070	−0.663445	3.055203
85	6	0	2.730964	−1.317472	2.002994
86	6	0	3.589160	−2.299473	1.366642
87	6	0	2.548593	3.080540	−1.271515
88	6	0	1.956981	2.743290	0.010765
89	6	0	2.716090	3.398610	1.065307
90	6	0	3.804023	4.110277	0.437480
91	6	0	3.704533	3.897993	−1.003955
92	6	0	5.321839	−0.041118	−3.297382
93	6	0	6.464734	0.802151	−3.047236
94	6	0	7.410052	0.053589	−2.253132

95	6	0	6.856142	−1.266283	−2.017831
96	6	0	5.559494	−1.326188	−2.665323
97	6	0	1.494086	0.457917	−0.808786
98	6	0	1.730846	−0.811076	−0.184259
99	6	0	1.824663	−0.591151	1.247515
100	6	0	1.626403	0.820255	1.509092
101	6	0	1.434278	1.473487	0.240776
102	6	0	3.299554	0.692037	3.305201
103	6	0	4.448976	1.537468	3.564173
104	6	0	4.207294	2.821639	2.933556
105	6	0	2.908425	2.761150	2.289775
106	6	0	2.351016	1.451719	2.523732
107	6	0	8.033324	2.319894	0.440925
108	6	0	8.271682	1.041876	1.068188
109	6	0	8.334653	0.031480	0.025889
110	6	0	8.134724	0.685710	−1.247830
111	6	0	7.933558	2.098612	−0.988776
112	6	0	5.251149	3.505865	2.331585
113	6	0	6.586481	2.941298	2.329300
114	6	0	7.203795	3.257349	1.054220
115	6	0	6.261276	4.017299	0.274047
116	6	0	5.051051	4.161587	1.051263
117	6	0	7.126283	−0.574994	2.521680
118	6	0	7.680337	0.738424	2.288854
119	6	0	6.816434	1.713629	2.928912
120	6	0	5.724678	0.996883	3.558672
121	6	0	5.916483	−0.418233	3.300092
122	3	0	4.102284	1.518874	−0.642086

$Li^+@C_{60}^-$ (doublet) by UωB97XD/6-31G(d)/SMD(oDCB)

E(UwB97XD) = −2293.07357328 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2292.737154 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.020658	0.425196	3.366062
2	6	0	2.261165	0.043799	2.715058
3	6	0	2.728295	1.173025	1.935490
4	6	0	1.764671	2.245113	2.094577
5	6	0	0.714606	1.780749	2.980810
6	6	0	−0.129818	3.478120	−0.652670
7	6	0	0.082250	3.459997	0.773429
8	6	0	1.456935	3.062048	1.017501
9	6	0	2.100257	2.847086	−0.263816
10	6	0	1.112996	3.093499	−1.296591
11	6	0	1.368137	−2.224325	2.380612
12	6	0	1.350690	−3.040176	1.201631
13	6	0	2.396963	−2.564542	0.310565
14	6	0	3.077951	−1.462263	0.958580
15	6	0	2.432874	−1.246254	2.238197
16	6	0	−0.172446	1.864331	−2.995869
17	6	0	1.093180	2.308085	−2.438500
18	6	0	2.060599	1.241223	−2.601357
19	6	0	1.381450	0.135238	−3.241167
20	6	0	0.003396	0.532482	−3.495795
21	6	0	−1.371045	2.241053	−2.378367
22	6	0	−2.427272	1.264821	−2.225863
23	6	0	−3.073269	1.485314	−0.943939
24	6	0	−2.394650	2.590603	−0.298496
25	6	0	−1.343515	3.052387	−1.187950
26	6	0	−0.000324	−0.513510	3.500710
27	6	0	−1.375906	−0.115133	3.256779
28	6	0	−2.056247	−1.220175	2.613791
29	6	0	−1.088235	−2.289692	2.448009
30	6	0	0.173325	−1.856476	3.010078
31	6	0	3.345510	0.967107	0.710401
32	6	0	3.522890	−0.380528	0.208774
33	6	0	3.312572	−0.356699	−1.221802
34	6	0	3.006607	1.000703	−1.608805
35	6	0	3.022959	1.821169	−0.415045
36	6	0	−0.604681	2.165002	2.747823
37	6	0	−0.925564	3.016092	1.627136
38	6	0	−2.189628	2.571908	1.072134
39	6	0	−2.655093	1.444816	1.857815
40	6	0	−1.667325	1.189829	2.889914
41	6	0	−3.515467	0.406162	−0.193382
42	6	0	−3.344973	−0.944020	−0.688212
43	6	0	−3.028316	−1.795276	0.429910
44	6	0	−2.999252	−0.977451	1.623927
45	6	0	−3.302659	0.387325	1.240003
46	6	0	0.935258	−3.003007	−1.629377
47	6	0	0.617512	−2.160106	−2.742804
48	6	0	1.678714	−1.169834	−2.874104
49	6	0	2.666311	−1.421580	−1.844903
50	6	0	2.200296	−2.546463	−1.062721
51	6	0	−2.102430	−2.831524	0.277555
52	6	0	−1.460402	−3.048829	−1.002653
53	6	0	−0.080791	−3.462738	−0.761291
54	6	0	0.130033	−3.467539	0.657887
55	6	0	−1.114307	−3.078084	1.304605
56	6	0	−1.019509	−0.414883	−3.353194
57	6	0	−0.721038	−1.771170	−2.989724
58	6	0	−1.769004	−2.226419	−2.085695
59	6	0	−2.732668	−1.153631	−1.924868
60	6	0	−2.263583	−0.029805	−2.703047
61	3	0	−0.149411	−1.000529	−0.699325

$Li^+@C_{60}^-$ dimer (singlet) by ωB97XD/6-31G(d)/SMD(oDCB)

E(RwB97XD) = −4586.18968171 au (*C*1 symmetry)

No imaginary frequency on IR calculation

Sum of electronic and thermal Free Energies= −4585.482480 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.942944	−0.809935	1.046002
2	6	0	7.464908	−2.085236	0.548513
3	6	0	7.422298	−2.012684	−0.900060
4	6	0	7.877758	−0.695035	−1.296982
5	6	0	8.192837	0.049432	−0.093803
6	6	0	5.719085	1.588779	−2.964608
7	6	0	6.980539	1.363021	−2.293534
8	6	0	7.278260	−0.055541	−2.371701
9	6	0	6.209721	−0.703864	−3.104429
10	6	0	5.239361	0.310075	−3.459877
11	6	0	5.913434	−2.217144	2.452739
12	6	0	4.503093	−2.540593	2.487008
13	6	0	4.190399	−3.260898	1.280389
14	6	0	5.407328	−3.420309	0.507218
15	6	0	6.480049	−2.774893	1.236987
16	6	0	2.953405	0.995348	−2.906249
17	6	0	3.882825	0.022792	−3.432691
18	6	0	3.417744	−1.300817	−3.039237
19	6	0	2.186986	−1.159543	−2.316871
20	6	0	1.915641	0.281270	−2.193361
21	6	0	3.408918	2.223662	−2.441053
22	6	0	2.855972	2.777164	−1.234834
23	6	0	3.931545	3.429652	−0.503208
24	6	0	5.148694	3.274791	−1.271559
25	6	0	4.824911	2.528195	−2.472693
26	6	0	7.404567	−0.280190	2.209403
27	6	0	7.107446	1.138407	2.288646
28	6	0	5.885217	1.295220	3.047356
29	6	0	5.429489	−0.026544	3.440204
30	6	0	6.376999	−1.000659	2.934201
31	6	0	6.398732	−2.634566	−1.596340
32	6	0	5.368203	−3.355553	−0.876485
33	6	0	4.108821	−3.118846	−1.560232
34	6	0	4.359151	−2.284087	−2.708757
35	6	0	5.768880	−1.963194	−2.719816
36	6	0	7.915010	1.406476	−0.019536
37	6	0	7.289673	2.075466	−1.143637
38	6	0	6.355620	3.053231	−0.622221
39	6	0	6.394343	2.978481	0.824739
40	6	0	7.354539	1.959721	1.197084
41	6	0	3.969052	3.362358	0.877321
42	6	0	2.933587	2.636901	1.599283
43	6	0	3.548603	1.972302	2.715495
44	6	0	4.965924	2.272861	2.696514
45	6	0	5.226329	3.132506	1.558040
46	6	0	2.035926	−2.053095	1.123404
47	6	0	1.364893	−1.434376	0.021375
48	6	0	1.962722	−1.943087	−1.169839
49	6	0	2.944046	−2.968443	−0.815647
50	6	0	2.986248	−3.038213	0.619183
51	6	0	3.115837	0.701721	3.078372
52	6	0	2.040326	0.059953	2.356697
53	6	0	2.321340	−1.384035	2.319762
54	6	0	3.585615	−1.593158	2.958493
55	6	0	4.073420	−0.312949	3.452436

56	6	0	1.364024	0.821270	−1.048141
57	6	0	0.785619	−0.026921	0.105878
58	6	0	1.420237	0.707465	1.306912
59	6	0	1.914757	1.996128	0.903017
60	6	0	1.879388	2.065950	−0.547132
61	3	0	3.399127	−0.364067	−0.160293
62	6	0	−1.962234	1.942207	−1.170063
63	6	0	−2.943261	2.967888	−0.815983
64	6	0	−2.985422	3.037860	0.618842
65	6	0	−2.035384	2.052525	1.123171
66	6	0	−1.364573	1.433466	0.021209
67	6	0	−3.115980	−0.701757	3.078513
68	6	0	−2.040300	−0.060377	2.356740
69	6	0	−2.320941	1.383685	2.319614
70	6	0	−3.585146	1.593239	2.958336
71	6	0	−4.073288	0.313226	3.452454
72	6	0	−4.358565	2.283651	−2.708969
73	6	0	−5.768380	1.963150	−2.719976
74	6	0	−6.398034	2.634840	−1.596578
75	6	0	−5.367303	3.355640	−0.876829
76	6	0	−4.107999	3.118511	−1.560570
77	6	0	−5.885533	−1.294495	3.047601
78	6	0	−5.429436	0.027192	3.440267
79	6	0	−6.376685	1.001504	2.934160
80	6	0	−7.404463	0.281224	2.209471
81	6	0	−7.107733	−1.137447	2.288891
82	6	0	−4.966512	−2.272430	2.696864
83	6	0	−5.227166	−3.132156	1.558510
84	6	0	−3.969961	−3.362435	0.877800
85	6	0	−2.934290	−2.637168	1.599650
86	6	0	−3.549111	−1.972256	2.715785
87	6	0	−2.186699	1.158572	−2.316990
88	6	0	−1.915735	−0.282307	−2.193304
89	6	0	−2.953715	−0.996193	−2.906078
90	6	0	−3.882878	−0.023445	−3.432626
91	6	0	−3.417433	1.300085	−3.039345
92	6	0	−4.189493	3.260979	1.280046
93	6	0	−5.406389	3.420594	0.506868
94	6	0	−6.479272	2.775555	1.236732
95	6	0	−5.912794	2.217805	2.452545
96	6	0	−4.502365	2.540879	2.486750
97	6	0	−0.785630	0.025895	0.105882
98	6	0	−1.420375	−0.708199	1.307038
99	6	0	−1.915274	−1.996776	0.903299
100	6	0	−1.879947	−2.066796	−0.546851
101	6	0	−1.364222	−0.822325	−1.048037
102	6	0	−3.932495	−3.429924	−0.502721
103	6	0	−5.149614	−3.274825	−1.271071
104	6	0	−4.825645	−2.528467	−2.472301
105	6	0	−3.409564	−2.224321	−2.440720
106	6	0	−2.856750	−2.777826	−1.234444
107	6	0	−7.877588	0.695755	−1.296958
108	6	0	−8.192845	−0.048473	−0.093680
109	6	0	−7.942711	0.810973	1.046012
110	6	0	−7.464325	2.086077	0.548356
111	6	0	−7.421761	2.013329	−0.900207
112	6	0	−5.719566	−1.588866	−2.964326
113	6	0	−6.980952	−1.362677	−2.293268
114	6	0	−7.278281	0.055959	−2.371606
115	6	0	−6.209573	0.703894	−3.104431
116	6	0	−5.239495	−0.310357	−3.459762
117	6	0	−7.355063	−1.958834	1.197436
118	6	0	−7.915390	−1.405584	−0.019246
119	6	0	−7.290259	−2.074890	−1.143272
120	6	0	−6.356470	−3.052849	−0.621744
121	6	0	−6.395149	−2.977905	0.825208
122	3	0	−3.399070	0.363593	−0.160365

$Li^{+}@C_{60}^{-}$ dimer (triplet) by UωB97XD/6-31G(d)/SMD(oDCB)

E(UwB97XD) = −4586.15709104 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4585.464234 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−8.229688	0.687243	1.322858
2	6	0	−8.223021	1.338197	0.027020
3	6	0	−8.352243	0.315876	−0.994010
4	6	0	−8.416637	−0.967446	−0.322781
5	6	0	−8.346817	−0.734339	1.107296
6	6	0	−5.896777	−3.442074	−0.759479
7	6	0	−7.064301	−3.001284	−0.035938
8	6	0	−7.792065	−2.071982	−0.880293
9	6	0	−7.074055	−1.941893	−2.132086
10	6	0	−5.895322	−2.783206	−2.051527
11	6	0	−6.568057	2.955931	0.865330
12	6	0	−5.335968	3.402391	0.279620
13	6	0	−5.406000	3.149853	−1.149341
14	6	0	−6.700560	2.572084	−1.447975
15	6	0	−7.416165	2.442470	−0.197026
16	6	0	−3.448825	−2.569180	−1.918439
17	6	0	−4.703643	−2.359606	−2.618846
18	6	0	−4.636837	−1.079406	−3.294166
19	6	0	−3.347336	−0.496209	−2.989945
20	6	0	−2.608430	−1.429922	−2.155396
21	6	0	−3.450220	−3.208019	−0.674599
22	6	0	−2.612276	−2.690599	0.388459
23	6	0	−3.328079	−2.827265	1.641857
24	6	0	−4.621297	−3.407586	1.343663
25	6	0	−4.691264	−3.641338	−0.087968
26	6	0	−7.410676	1.175870	2.339383
27	6	0	−6.683969	0.246496	3.186187
28	6	0	−5.391121	0.827131	3.485515
29	6	0	−5.320347	2.106562	2.806765
30	6	0	−6.574403	2.325283	2.113012
31	6	0	−7.666681	0.439312	−2.193384
32	6	0	−6.820379	1.591913	−2.426500
33	6	0	−5.653442	1.153757	−3.156255
34	6	0	−5.766843	−0.270134	−3.368290
35	6	0	−7.013315	−0.715791	−2.777714
36	6	0	−7.648323	−1.627041	1.917741
37	6	0	−6.998044	−2.777498	1.336952
38	6	0	−5.745535	−2.987520	2.037198
39	6	0	−5.623076	−1.964246	3.057693
40	6	0	−6.799328	−1.119148	2.977506
41	6	0	−3.210981	−1.849307	2.619891
42	6	0	−2.367715	−0.695217	2.396525
43	6	0	−3.015194	0.455653	2.979846
44	6	0	−4.265066	0.017737	3.562241
45	6	0	−4.385558	−1.411343	3.347397
46	6	0	−3.011481	2.539466	−1.160170
47	6	0	−2.365315	1.396506	−1.738273
48	6	0	−3.230999	0.874878	−2.791943
49	6	0	−4.407222	1.715788	−2.873062
50	6	0	−4.281772	2.736269	−1.853607
51	6	0	−2.949333	1.691459	2.334284
52	6	0	−2.233638	1.822306	1.082063
53	6	0	−2.951796	2.770656	0.234827
54	6	0	−4.119705	3.192789	0.950497
55	6	0	−4.124029	2.530964	2.247415
56	6	0	−1.794060	−0.929841	−1.127862
57	6	0	−1.661975	0.481998	−0.917964
58	6	0	−1.614249	0.711502	0.520558
59	6	0	−1.677615	−0.570522	1.192228
60	6	0	−1.803910	−1.584921	0.171378
61	3	0	−4.042123	0.601521	−0.265639
62	6	0	3.423340	3.244821	−0.595211
63	6	0	4.750199	3.523610	−1.073190
64	6	0	4.913900	2.835610	−2.348854
65	6	0	3.670635	2.157567	−2.668912
66	6	0	2.752904	2.400401	−1.579587
67	6	0	3.500933	−1.404280	−2.928895
68	6	0	2.795566	−0.137577	−2.857832
69	6	0	3.698082	0.904067	−3.300876
70	6	0	4.957237	0.293631	−3.632582
71	6	0	4.842771	−1.134685	−3.406594
72	6	0	5.588913	3.329310	1.247383
73	6	0	6.709780	2.584648	1.788139
74	6	0	7.629707	2.335628	0.698847
75	6	0	7.081109	2.942244	−0.504057
76	6	0	5.835866	3.562857	−0.167079
77	6	0	5.695572	−2.858634	−1.879610
78	6	0	5.914247	−1.847591	−2.892558
79	6	0	7.158921	−1.167176	−2.573902
80	6	0	7.712668	−1.766861	−1.382007
81	6	0	6.806127	−2.802869	−0.946180
82	6	0	4.412476	−3.118427	−1.421831
83	6	0	4.172564	−3.332356	−0.008549
84	6	0	2.909562	−2.720739	0.330430
85	6	0	2.365715	−2.122209	−0.870118
86	6	0	3.292895	−2.369875	−1.958034
87	6	0	3.185830	3.025684	0.771735

88	6	0	2.289128	1.994817	1.199154
89	6	0	2.843888	1.388438	2.396137
90	6	0	4.084419	2.065181	2.720588
91	6	0	4.305462	3.072021	1.706565
92	6	0	6.131572	2.232854	−2.667057
93	6	0	7.249722	2.295507	−1.740984
94	6	0	7.942729	1.037530	−1.808364
95	6	0	7.270288	0.200440	−2.788916
96	6	0	6.157226	0.945174	−3.331806
97	6	0	1.889382	1.393047	−1.153417
98	6	0	1.909296	0.098852	−1.816878
99	6	0	1.692287	−0.911325	−0.804047
100	6	0	1.539102	−0.236007	0.471150
101	6	0	1.640175	1.184138	0.251200
102	6	0	2.754422	−2.071060	1.555475
103	6	0	3.865724	−2.015518	2.487638
104	6	0	3.841739	−0.725696	3.149657
105	6	0	2.729525	0.022900	2.607207
106	6	0	2.056518	−0.814064	1.625597
107	6	0	8.091563	0.115449	1.638062
108	6	0	8.111624	−1.175826	0.976401
109	6	0	8.353330	−0.958275	−0.436640
110	6	0	8.473024	0.456975	−0.654797
111	6	0	8.303851	1.127540	0.624520
112	6	0	5.034751	−0.077761	3.455208
113	6	0	6.299250	−0.695220	3.113744
114	6	0	7.204706	0.350111	2.680100
115	6	0	6.498268	1.611679	2.757155
116	6	0	5.157815	1.346183	3.236534
117	6	0	6.574478	−3.011550	0.408879
118	6	0	7.243285	−2.174083	1.390250
119	6	0	6.319469	−1.929552	2.477500
120	6	0	5.076661	−2.605369	2.160431
121	6	0	5.238614	−3.279823	0.886230
122	3	0	4.864753	1.170272	−0.627003

C_{60}^- (doublet) by UM06-2x/6-31G(d) without solvent parameters

E(UM062X) = −2285.53476910 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2285.204442 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.350871	3.322144	1.182169
2	6	0	−1.693756	3.014146	0.726751
3	6	0	−1.694744	3.024813	−0.726556
4	6	0	0.477138	3.501168	0.004841
5	6	0	−0.361088	3.323359	−1.170245
6	6	0	0.165276	2.695773	2.310970
7	6	0	1.535960	2.222214	2.311191
8	6	0	1.574493	0.967149	3.035789
9	6	0	−0.640616	1.733592	3.036257
10	6	0	0.230544	0.666159	3.484026
11	6	0	−2.465817	2.093771	1.421723
12	6	0	−1.928920	1.440800	2.599628
13	6	0	−2.401434	0.068927	2.589146
14	6	0	−3.282066	1.129278	0.699811
15	6	0	−3.244607	−0.114141	1.418971
16	6	0	−2.480495	2.094331	−1.419303
17	6	0	−3.278587	1.139862	−0.700043
18	6	0	−3.232581	−0.122832	−1.421547
19	6	0	−1.930486	1.429369	−2.589287
20	6	0	−2.406818	0.058953	−2.599445
21	6	0	1.788880	3.047564	0.004904
22	6	0	2.338377	2.390839	−1.170577
23	6	0	3.202909	1.332054	−0.726727
24	6	0	2.329517	2.396339	1.182514
25	6	0	3.195479	1.324211	0.727007
26	6	0	0.169506	2.687816	−2.299662
27	6	0	−0.642222	1.718011	−3.018430
28	6	0	0.224970	0.649688	−3.476027
29	6	0	1.527846	2.218472	−2.299625
30	6	0	1.566301	0.953653	−3.017719
31	6	0	0.350871	−3.322144	−1.182169
32	6	0	−0.477138	−3.501168	−0.004841
33	6	0	0.361088	−3.323359	1.170245
34	6	0	1.693756	−3.014146	−0.726751
35	6	0	1.694744	−3.024813	0.726556
36	6	0	−0.165276	−2.695773	−2.310970
37	6	0	0.640616	−1.733592	−3.036257
38	6	0	−0.230544	−0.666159	−3.484026
39	6	0	−1.535960	−2.222214	−2.311191
40	6	0	−1.574493	−0.967149	−3.035789
41	6	0	−1.788880	−3.047564	−0.004904
42	6	0	−2.329517	−2.396339	−1.182514
43	6	0	−3.195479	−1.324211	−0.727007
44	6	0	−2.338377	−2.390839	1.170577
45	6	0	−3.202909	−1.332054	0.726727
46	6	0	−0.169506	−2.687816	2.299662
47	6	0	−1.527846	−2.218472	2.299625
48	6	0	−1.566301	−0.953653	3.017719
49	6	0	0.642222	−1.718011	3.018430
50	6	0	−0.224970	−0.649688	3.476027
51	6	0	2.465817	−2.093771	−1.421723
52	6	0	3.282066	−1.129278	−0.699811
53	6	0	3.244607	0.114141	−1.418971
54	6	0	1.928920	−1.440800	−2.599628
55	6	0	2.401434	−0.068927	−2.589146
56	6	0	2.480495	−2.094331	1.419303
57	6	0	1.930486	−1.429369	2.589287
58	6	0	2.406818	−0.058953	2.599445
59	6	0	3.278587	−1.139862	0.700043
60	6	0	3.232581	0.122832	1.421547

C_{60}^- dimer (singlet) by M06-2x/6-31G(d) without solvent parameters

E(RM062X) = −4571.03676722 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4570.341959 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.893868	0.763188	−1.174402
2	6	0	7.426440	2.063841	−0.726581
3	6	0	7.426439	2.063940	0.726301
4	6	0	7.893871	0.763350	1.174299
5	6	0	8.175888	−0.039593	0.000003
6	6	0	5.785140	−1.442493	3.015510
7	6	0	7.027376	−1.248125	2.297760
8	6	0	7.320324	0.176708	2.296367
9	6	0	6.276388	0.859120	3.033018
10	6	0	5.316660	−0.139201	3.460507
11	6	0	5.814623	2.098962	−2.592197
12	6	0	4.409906	2.420976	−2.604014
13	6	0	4.125337	3.206041	−1.423453
14	6	0	5.366255	3.405886	−0.694158
15	6	0	6.416614	2.716083	−1.419482
16	6	0	3.011510	−0.853130	3.000394
17	6	0	3.956427	0.144076	3.443238
18	6	0	3.474680	1.449820	2.999465
19	6	0	2.231863	1.270987	2.319380
20	6	0	1.956511	−0.172672	2.281899
21	6	0	3.457308	−2.108514	2.587764
22	6	0	2.872997	−2.719311	1.425377
23	6	0	3.929662	−3.404262	0.692795
24	6	0	5.170692	−3.206893	1.416872
25	6	0	4.875676	−2.404496	2.591584
26	6	0	7.320321	0.176392	−2.296389
27	6	0	7.027372	−1.248440	−2.297585
28	6	0	5.785135	−1.442907	−3.015307
29	6	0	5.316654	−0.139677	−3.460482
30	6	0	6.276382	0.858705	−3.033129
31	6	0	6.416612	2.716276	1.419113
32	6	0	5.366255	3.405981	0.693695
33	6	0	4.125338	3.206236	1.423019
34	6	0	4.409909	2.421334	2.603691
35	6	0	5.814624	2.099317	2.591914
36	6	0	7.903476	−1.404385	0.000098
37	6	0	7.310095	−2.016508	1.173431
38	6	0	6.361918	−3.019738	0.725925
39	6	0	6.361917	−3.019837	−0.725507
40	6	0	7.310091	−2.016668	−1.173150
41	6	0	3.929661	−3.404359	−0.692320
42	6	0	2.872997	−2.719504	−1.424994
43	6	0	3.457304	−2.108869	−2.587467
44	6	0	4.875672	−2.404853	−2.591249
45	6	0	5.170690	−3.207089	−1.416427
46	6	0	1.979828	1.995060	−1.141902
47	6	0	1.351084	1.439206	−0.000092
48	6	0	1.979830	1.995214	1.141636
49	6	0	2.945777	3.011521	0.718262

50	6	0	2.945776	3.011423	−0.718668
51	6	0	3.011504	−0.853541	−3.000269
52	6	0	1.956507	−0.172987	−2.281863
53	6	0	2.231862	1.270669	−2.319540
54	6	0	3.474679	1.449409	−2.999657
55	6	0	3.956422	0.143604	−3.443251
56	6	0	1.380870	−0.765010	1.178137
57	6	0	0.791090	0.028670	0.000005
58	6	0	1.380867	−0.765172	−1.178019
59	6	0	1.880751	−2.031768	−0.726796
60	6	0	1.880752	−2.031668	0.727087
61	6	0	−1.979830	−1.995047	1.141930
62	6	0	−2.945779	−3.011416	0.718703
63	6	0	−2.945775	−3.011529	−0.718227
64	6	0	−1.979828	−1.995228	−1.141608
65	6	0	−1.351084	−1.439206	0.000122
66	6	0	−3.011498	0.853099	−3.000397
67	6	0	−1.956502	0.172650	−2.281890
68	6	0	−2.231858	−1.271011	−2.319352
69	6	0	−3.474672	−1.449851	−2.999448
70	6	0	−3.956415	−0.144112	−3.443234
71	6	0	−4.409915	−2.420950	2.604040
72	6	0	−5.814630	−2.098935	2.592213
73	6	0	−6.416618	−2.716068	1.419502
74	6	0	−5.366257	−3.405878	0.694188
75	6	0	−4.125342	−3.206024	1.423485
76	6	0	−5.785128	1.442463	−3.015528
77	6	0	−5.316647	0.139167	−3.460512
78	6	0	−6.276376	−0.859150	−3.033014
79	6	0	−7.320317	−0.176730	−2.296375
80	6	0	−7.027368	1.248102	−2.297783
81	6	0	−4.875666	2.404470	−2.591609
82	6	0	−5.170687	3.206879	−1.416906
83	6	0	−3.929659	3.404257	−0.692826
84	6	0	−2.872992	2.719295	−1.425396
85	6	0	−3.457298	2.108487	−2.587780
86	6	0	−2.231867	−1.270646	2.319567
87	6	0	−1.956516	0.173008	2.281872
88	6	0	−3.011516	0.853571	3.000267
89	6	0	−3.956435	−0.143569	3.443255
90	6	0	−3.474687	−1.449378	2.999674
91	6	0	−4.125334	−3.206253	−1.422987
92	6	0	−5.366253	−3.405989	−0.693666
93	6	0	−6.416609	−2.716291	−1.419094
94	6	0	−5.814617	−2.099344	−2.591899
95	6	0	−4.409900	−2.421360	−2.603664
96	6	0	−0.791090	−0.028671	0.000010
97	6	0	−1.380866	0.764997	−1.178131
98	6	0	−1.880749	2.031661	−0.727096
99	6	0	−1.880754	2.031775	0.726787
100	6	0	−1.380870	0.765184	1.178025
101	6	0	−3.929663	3.404364	0.692289
102	6	0	−5.170695	3.207103	1.416393
103	6	0	−4.875682	2.404879	2.591224
104	6	0	−3.457313	2.108896	2.587451
105	6	0	−2.873001	2.719520	1.424974
106	6	0	−7.893874	−0.763176	1.174397
107	6	0	−8.175888	0.039594	−0.000017
108	6	0	−7.893866	−0.763362	−1.174303
109	6	0	−7.426437	−2.063948	−0.726291
110	6	0	−7.426443	−2.063833	0.726591
111	6	0	−5.785146	1.442937	3.015288
112	6	0	−7.027379	1.248463	2.297562
113	6	0	−7.320329	−0.176370	2.296380
114	6	0	−6.276394	−0.858674	3.033133
115	6	0	−5.316667	0.139711	3.460478
116	6	0	−7.310090	2.016496	−1.173461
117	6	0	−7.903475	1.404385	−0.000124
118	6	0	−7.310095	2.016680	1.173120
119	6	0	−6.361919	3.019845	0.725470
120	6	0	−6.361915	3.019731	−0.725962

C_{60}^- dimer (triplet) by UM06-2x/6-31G(d) without solvent parameters

E(UM062X) = −4571.02964045 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4570.350086 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.246408	1.462938	−0.235259
2	6	0	8.294159	0.867002	1.083965
3	6	0	8.421850	−0.568362	0.923937
4	6	0	8.453887	−0.859251	−0.496379
5	6	0	8.345076	0.397482	−1.212017
6	6	0	5.882968	−2.790548	−2.065351
7	6	0	7.041469	−1.926210	−2.210775
8	6	0	7.817496	−1.994508	−0.985970
9	6	0	7.119813	−2.888318	−0.080112
10	6	0	5.930669	−3.381904	−0.755019
11	6	0	6.625490	2.510203	1.853778
12	6	0	5.403979	2.322359	2.618075
13	6	0	5.512081	1.074975	3.326449
14	6	0	6.804898	0.485885	3.009429
15	6	0	7.501702	1.381186	2.107521
16	6	0	3.480495	−3.152615	−0.589874
17	6	0	4.753160	−3.566741	−0.018965
18	6	0	4.721673	−3.277047	1.389265
19	6	0	3.428161	−2.684065	1.698089
20	6	0	2.653289	−2.620620	0.475453
21	6	0	3.434929	−2.581186	−1.854178
22	6	0	2.558730	−1.453019	−2.108371
23	6	0	3.255502	−0.557734	−3.009778
24	6	0	4.549515	−1.146071	−3.325950
25	6	0	4.657585	−2.393197	−2.618029
26	6	0	7.407171	2.548943	−0.477026
27	6	0	6.632170	2.612722	−1.700085
28	6	0	5.339789	3.206528	−1.391216
29	6	0	5.308311	3.496241	0.017549
30	6	0	6.579788	3.081516	0.588710
31	6	0	7.755233	−1.427238	1.791556
32	6	0	6.927435	−0.889090	2.856939
33	6	0	5.769431	−1.751345	3.015025
34	6	0	5.866734	−2.807193	2.042966
35	6	0	7.089315	−2.609459	1.279856
36	6	0	7.602163	0.460866	−2.387198
37	6	0	6.937192	−0.722525	−2.895371
38	6	0	5.665174	−0.315121	−3.473244
39	6	0	5.537847	1.109019	−3.317945
40	6	0	6.726338	1.591786	−2.637046
41	6	0	3.133132	0.816366	−2.856843
42	6	0	2.304729	1.355169	−1.792731
43	6	0	2.970924	2.536340	−1.280626
44	6	0	4.195037	2.733360	−2.042710
45	6	0	4.292340	1.678091	−3.014665
46	6	0	3.123315	0.650273	2.892774
47	6	0	2.458266	−0.532883	2.385281
48	6	0	3.334275	−1.663249	2.634131
49	6	0	4.523798	−1.180545	3.314776
50	6	0	4.396531	0.243177	3.469649
51	6	0	2.940467	2.815003	0.078578
52	6	0	2.242511	1.922422	0.984414
53	6	0	3.019132	1.853066	2.208330
54	6	0	4.178857	2.716702	2.062809
55	6	0	4.131154	3.307686	0.752925
56	6	0	1.814679	−1.534824	0.233684
57	6	0	1.716742	−0.469334	1.210257
58	6	0	1.606746	0.787481	0.494890
59	6	0	1.638553	0.496642	−0.925386
60	6	0	1.766772	−0.938978	−1.085291
61	6	0	−3.335866	1.670355	2.631839
62	6	0	−4.526168	1.189943	3.312994
63	6	0	−4.399354	−0.233340	3.472241
64	6	0	−3.125830	−0.642357	2.897447
65	6	0	−2.459977	0.539104	2.387070
66	6	0	−2.941337	−2.815360	0.089758
67	6	0	−2.243945	−1.920373	0.993479
68	6	0	−3.021509	−1.847205	2.216582
69	6	0	−4.181286	−2.711013	2.072924
70	6	0	−4.132834	−3.305662	0.764674
71	6	0	−5.867678	2.813440	2.035665
72	6	0	−7.089544	2.613615	1.272209
73	6	0	−7.756277	1.433029	1.786908
74	6	0	−6.929545	0.897805	2.854461
75	6	0	−5.771297	1.760233	3.010688
76	6	0	−5.339735	−3.210741	−1.380688
77	6	0	−5.309350	−3.496042	0.029009
78	6	0	−6.581254	−3.079494	0.598128
79	6	0	−7.407579	−2.549880	−0.469753
80	6	0	−6.631574	−2.617428	−1.692142
81	6	0	−4.194229	−2.739819	−2.032723
82	6	0	−4.290585	−1.687207	−3.007656
83	6	0	−3.131135	−0.825325	−2.851676

84	6	0	−2.303773	−1.361222	−1.785393
85	6	0	−2.970820	−2.540722	−1.270282
86	6	0	−3.428877	2.688520	1.692843
87	6	0	−2.653018	2.621290	0.470881
88	6	0	−3.479155	3.150340	−0.596592
89	6	0	−4.752243	3.566299	−0.027723
90	6	0	−4.721853	3.281028	1.381414
91	6	0	−5.515072	−1.065264	3.330766
92	6	0	−6.807429	−0.476723	3.011166
93	6	0	−7.503783	−1.374442	2.111205
94	6	0	−6.627690	−2.504578	1.861527
95	6	0	−5.406783	−2.314763	2.626125
96	6	0	−1.717580	0.471889	1.212690
97	6	0	−1.607341	−0.787004	0.501137
98	6	0	−1.638071	−0.500430	−0.919968
99	6	0	−1.765846	0.934811	−1.084239
100	6	0	−1.814532	1.534580	0.233038
101	6	0	−3.253076	0.548324	−3.008804
102	6	0	−4.546642	1.136130	−3.327557
103	6	0	−4.654896	2.385352	−2.623405
104	6	0	−3.432858	2.575282	−1.859212
105	6	0	−2.556736	1.446029	−2.109364
106	6	0	−8.453389	0.858498	−0.499897
107	6	0	−8.344411	−0.400291	−1.211744
108	6	0	−8.246655	−1.462948	−0.231901
109	6	0	−8.295197	−0.863101	1.085637
110	6	0	−8.422458	0.571894	0.921237
111	6	0	−5.880674	2.784615	−2.072765
112	6	0	−7.039225	1.920097	−2.216311
113	6	0	−7.816256	1.992242	−0.992348
114	6	0	−7.119075	2.888408	−0.088603
115	6	0	−5.929122	3.379631	−0.764103
116	6	0	−6.724865	−1.599130	−2.632042
117	6	0	−7.600560	−0.467324	−2.386255
118	6	0	−6.934799	0.714361	−2.897334
119	6	0	−5.662482	0.305035	−3.473152
120	6	0	−5.535599	−1.118646	−3.313465

C_{60}^- (doublet) by UM06-2x/6-31G(d)/IEFPCM(oDCB)

E(UM062X) = −2285.57734628 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2285.246933 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.350871	3.322144	1.182169
2	6	0	−1.693756	3.014146	0.726751
3	6	0	−1.694744	3.024813	−0.726556
4	6	0	0.477138	3.501168	0.004841
5	6	0	−0.361088	3.323359	−1.170245
6	6	0	0.165276	2.695773	2.310970
7	6	0	1.535960	2.222214	2.311191
8	6	0	1.574493	0.967149	3.035789
9	6	0	−0.640616	1.733592	3.036257
10	6	0	0.230544	0.666159	3.484026
11	6	0	−2.465817	2.093771	1.421723
12	6	0	−1.928920	1.440800	2.599628
13	6	0	−2.401434	0.068927	2.589146
14	6	0	−3.282066	1.129278	0.699811
15	6	0	−3.244607	−0.114141	1.418971
16	6	0	−2.480495	2.094331	−1.419303
17	6	0	−3.278587	1.139862	−0.700043
18	6	0	−3.232581	−0.122832	−1.421547
19	6	0	−1.930486	1.429369	−2.589287
20	6	0	−2.406818	0.058953	−2.599445
21	6	0	1.788880	3.047564	0.004904
22	6	0	2.338377	2.390839	−1.170577
23	6	0	3.202909	1.332054	−0.726727
24	6	0	2.329517	2.396339	1.182514
25	6	0	3.195479	1.324211	0.727007
26	6	0	0.169506	2.687816	−2.299662
27	6	0	−0.642222	1.718011	−3.018430
28	6	0	0.224970	0.649688	−3.476027
29	6	0	1.527846	2.218472	−2.299625
30	6	0	1.566301	0.953653	−3.017719
31	6	0	0.350871	−3.322144	−1.182169
32	6	0	−0.477138	−3.501168	−0.004841
33	6	0	0.361088	−3.323359	1.170245
34	6	0	1.693756	−3.014146	−0.726751
35	6	0	1.694744	−3.024813	0.726556
36	6	0	−0.165276	−2.695773	−2.310970
37	6	0	0.640616	−1.733592	−3.036257
38	6	0	−0.230544	−0.666159	−3.484026
39	6	0	−1.535960	−2.222214	−2.311191
40	6	0	−1.574493	−0.967149	−3.035789
41	6	0	−1.788880	−3.047564	−0.004904
42	6	0	−2.329517	−2.396339	−1.182514
43	6	0	−3.195479	−1.324211	−0.727007
44	6	0	−2.338377	−2.390839	1.170577
45	6	0	−3.202909	−1.332054	0.726727
46	6	0	−0.169506	−2.687816	2.299662
47	6	0	−1.527846	−2.218472	2.299625
48	6	0	−1.566301	−0.953653	3.017719
49	6	0	0.642222	−1.718011	3.018430
50	6	0	−0.224970	−0.649688	3.476027
51	6	0	2.465817	−2.093771	−1.421723
52	6	0	3.282066	−1.129278	−0.699811
53	6	0	3.244607	0.114141	−1.418971
54	6	0	1.928920	−1.440800	−2.599628
55	6	0	2.401434	−0.068927	−2.589146
56	6	0	2.480495	−2.094331	1.419303
57	6	0	1.930486	−1.429369	2.589287
58	6	0	2.406818	−0.058953	2.599445
59	6	0	3.278587	−1.139862	0.700043
60	6	0	3.232581	0.122832	1.421547

C_{60}^- dimer (singlet) by M06-2x/6-31G(d)/IEFPCM(oDCB)

E(RM062X) = -4571.17103988 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4570.475596 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−7.891878	−0.762033	−1.174150
2	6	0	−7.424788	−2.062367	−0.726449
3	6	0	−7.424706	−2.062529	0.726259
4	6	0	−7.891776	−0.762302	1.174316
5	6	0	−8.174555	0.040645	0.000192
6	6	0	−5.783002	1.442266	3.015090
7	6	0	−7.025545	1.248234	2.297616
8	6	0	−7.319456	−0.175760	2.296137
9	6	0	−6.274105	−0.858787	3.030992
10	6	0	−5.314414	0.138919	3.459362
11	6	0	−5.814769	−2.098282	−2.591924
12	6	0	−4.408750	−2.420097	−2.603656
13	6	0	−4.124901	−3.204639	−1.423245
14	6	0	−5.365986	−3.404676	−0.694147
15	6	0	−6.416391	−2.715658	−1.419641
16	6	0	−3.009876	0.851919	3.000336
17	6	0	−3.954575	−0.145212	3.444466
18	6	0	−3.473776	−1.450418	3.000124
19	6	0	−2.228538	−1.272858	2.320866
20	6	0	−1.954662	0.171578	2.281808
21	6	0	−3.455853	2.106883	2.587278
22	6	0	−2.871802	2.717580	1.424643
23	6	0	−3.928424	3.404135	0.692744
24	6	0	−5.168729	3.207342	1.417411
25	6	0	−4.874120	2.404076	2.591443
26	6	0	−7.319697	−0.175227	−2.295904
27	6	0	−7.025769	1.248754	−2.297081
28	6	0	−5.783310	1.442960	−3.014640
29	6	0	−5.314754	0.139732	−3.459248
30	6	0	−6.274399	−0.858088	−3.031001
31	6	0	−6.416229	−2.715975	1.419188
32	6	0	−5.365909	−3.404824	0.693420
33	6	0	−4.124744	−3.204943	1.422430
34	6	0	−4.408484	−2.420700	2.603099
35	6	0	−5.814472	−2.098862	2.591549
36	6	0	−7.900112	1.404003	0.000331
37	6	0	−7.307465	2.016488	1.173719
38	6	0	−6.359093	3.019075	0.726007
39	6	0	−6.359170	3.019242	−0.725138
40	6	0	−7.307572	2.016748	−1.172975
41	6	0	−3.928500	3.404310	−0.692035
42	6	0	−2.871953	2.717894	−1.424191
43	6	0	−3.456112	2.107470	−2.586900
44	6	0	−4.874377	2.404680	−2.590864
45	6	0	−5.168867	3.207680	−1.416617
46	6	0	−1.979382	−1.995358	−1.142119
47	6	0	−1.347913	−1.440559	−0.000310

48	6	0	−1.979241	−1.995596	1.141365
49	6	0	−2.944376	−3.012226	0.717964
50	6	0	−2.944464	−3.012054	−0.718848
51	6	0	−3.010167	0.852611	−3.000301
52	6	0	−1.954885	0.172120	−2.282018
53	6	0	−2.228860	−1.272300	−2.321292
54	6	0	−3.474115	−1.449735	−3.000582
55	6	0	−3.954922	−0.144414	−3.444571
56	6	0	−1.379105	0.763977	1.177832
57	6	0	−0.789323	−0.029236	−0.000187
58	6	0	−1.379208	0.764250	−1.177972
59	6	0	−1.879149	2.031190	−0.726907
60	6	0	−1.879085	2.031007	0.727112
61	6	0	1.979243	1.995427	1.141660
62	6	0	2.944376	3.012120	0.718406
63	6	0	2.944461	3.012159	−0.718406
64	6	0	1.979379	1.995525	−1.141824
65	6	0	1.347912	1.440557	−0.000097
66	6	0	3.010162	−0.852170	−3.000429
67	6	0	1.954881	−0.171785	−2.282045
68	6	0	2.228854	1.272641	−2.321106
69	6	0	3.474107	1.450176	−3.000372
70	6	0	3.954914	0.144921	−3.444553
71	6	0	4.408489	2.420316	2.603448
72	6	0	5.814478	2.098480	2.591848
73	6	0	6.416233	2.715768	1.419577
74	6	0	5.365909	3.404722	0.693914
75	6	0	4.124747	3.204733	1.422897
76	6	0	5.783303	−1.442516	−3.014862
77	6	0	5.314746	−0.139222	−3.459278
78	6	0	6.274392	0.858534	−3.030886
79	6	0	7.319692	0.175566	−2.295890
80	6	0	7.025766	−1.248416	−2.297278
81	6	0	4.874372	−2.404297	−2.591224
82	6	0	5.168866	−3.207469	−1.417096
83	6	0	3.928500	−3.404208	−0.692540
84	6	0	2.871949	−2.717687	−1.424593
85	6	0	3.456107	−2.107089	−2.587213
86	6	0	2.228543	1.272515	2.321052
87	6	0	1.954667	−0.171916	2.281782
88	6	0	3.009882	−0.852361	3.000209
89	6	0	3.954582	0.144704	3.444483
90	6	0	3.473784	1.449975	3.000334
91	6	0	4.124896	3.204849	−1.422779
92	6	0	5.365982	3.404779	−0.693654
93	6	0	6.416384	2.715867	−1.419251
94	6	0	5.814761	2.098664	−2.591625
95	6	0	4.408742	2.420481	−2.603307
96	6	0	0.789323	0.029234	−0.000182
97	6	0	1.379208	−0.764077	−1.178084
98	6	0	1.879147	−2.031084	−0.727206
99	6	0	1.879089	−2.031116	0.726813
100	6	0	1.379105	−0.764153	1.177720
101	6	0	3.928427	−3.404238	0.692239
102	6	0	5.168733	−3.207552	1.416931
103	6	0	4.874127	−2.404458	2.591083
104	6	0	3.455859	−2.107264	2.586965
105	6	0	2.871808	−2.717790	1.424241
106	6	0	7.891778	0.762130	1.174414
107	6	0	8.174555	−0.040644	0.000171
108	6	0	7.891875	0.762208	−1.174052
109	6	0	7.424784	2.062474	−0.726159
110	6	0	7.424708	2.062424	0.726549
111	6	0	5.783010	−1.442709	3.014868
112	6	0	7.025550	−1.248571	2.297419
113	6	0	7.319461	0.175423	2.296151
114	6	0	6.274110	0.858342	3.031107
115	6	0	5.314422	−0.139429	3.459333
116	6	0	7.307572	−2.016575	−1.173286
117	6	0	7.900113	−1.404002	0.000109
118	6	0	7.307467	−2.016659	1.173408
119	6	0	6.359096	−3.019181	0.725552
120	6	0	6.359170	−3.019134	−0.725592

C_{60}^- dimer (triplet) by UM06-2x/6-31G(d)/IEFPCM(oDCB)

E(UM062X) = −4571.15745850 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4570.481233 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−8.380221	0.019113	−0.164604
2	6	0	−8.177415	−0.638502	−1.427225
3	6	0	−8.037395	−2.060847	−1.175438
4	6	0	−8.170897	−2.285554	0.253397
5	6	0	−8.372498	−0.993056	0.880054
6	6	0	−5.483277	−3.591493	2.195318
7	6	0	−6.794743	−2.972963	2.171488
8	6	0	−7.398921	−3.254188	0.882982
9	6	0	−6.458964	−4.046309	0.113666
10	6	0	−5.277467	−4.253842	0.924423
11	6	0	−6.777527	1.254432	−2.159032
12	6	0	−5.465698	1.275018	−2.782086
13	6	0	−5.261674	−0.016182	−3.404246
14	6	0	−6.455630	−0.820804	−3.180422
15	6	0	−7.390404	−0.035465	−2.419715
16	6	0	−2.914849	−3.555969	0.980028
17	6	0	−4.016257	−4.237032	0.330150
18	6	0	−3.887292	−4.009074	−1.095178
19	6	0	−2.693037	−3.210559	−1.324946
20	6	0	−2.093958	−2.931373	−0.046684
21	6	0	−3.111167	−2.919688	2.198938
22	6	0	−2.498713	−1.629527	2.459206
23	6	0	−3.434109	−0.843780	3.220389
24	6	0	−4.627908	−1.647900	3.443309
25	6	0	−4.423538	−2.939503	2.820846
26	6	0	−7.796054	1.266267	0.086702
27	6	0	−7.197171	1.545052	1.363802
28	6	0	−6.002426	2.344359	1.134113
29	6	0	−5.873428	2.572535	−0.290515
30	6	0	−6.974203	1.890650	−0.940106
31	6	0	−7.136748	−2.819802	−1.911350
32	6	0	−6.322560	−2.192004	−2.942846
33	6	0	−5.022303	−2.806617	−2.922529
34	6	0	−5.019940	−3.810264	−1.873553
35	6	0	−6.334320	−3.831249	−1.256298
36	6	0	−7.794408	−0.723367	2.112547
37	6	0	−6.990497	−1.734919	2.771766
38	6	0	−5.883401	−1.055189	3.421040
39	6	0	−6.018440	0.369301	3.179047
40	6	0	−7.191010	0.574006	2.371779
41	6	0	−3.567242	0.526760	2.981878
42	6	0	−2.751733	1.155421	1.951750
43	6	0	−3.554858	2.165920	1.295994
44	6	0	−4.869779	2.144383	1.912206
45	6	0	−4.867810	1.141258	2.961634
46	6	0	−2.899060	0.069733	−2.732163
47	6	0	−2.095172	−0.941991	−2.073404
48	6	0	−2.699789	−2.239215	−2.331590
49	6	0	−3.871861	−2.034362	−3.139651
50	6	0	−4.006489	−0.609674	−3.381156
51	6	0	−3.430414	2.380765	−0.073851
52	6	0	−2.489796	1.588803	−0.843057
53	6	0	−3.094243	1.307678	−2.131841
54	6	0	−4.405534	1.926214	−2.155243
55	6	0	−4.611405	2.588560	−0.884793
56	6	0	−1.511247	−1.685120	0.204148
57	6	0	−1.521516	−0.673178	−0.839949
58	6	0	−1.720448	0.619551	−0.212957
59	6	0	−1.850512	0.396349	1.216432
60	6	0	−1.712062	−1.026611	1.467913
61	6	0	2.728151	2.241523	−2.379342
62	6	0	3.910828	2.039579	−3.172890
63	6	0	4.050064	0.616137	−3.416059
64	6	0	2.935264	−0.066005	−2.782277
65	6	0	2.121225	0.943600	−2.131987
66	6	0	3.435530	−2.381924	−0.121955
67	6	0	2.503710	−1.589042	−0.901162
68	6	0	3.124344	−1.304131	−2.181755
69	6	0	4.436732	−1.921593	−2.189200
70	6	0	4.626512	−2.586873	−0.917973
71	6	0	5.040881	3.813441	−1.887489
72	6	0	6.347628	3.834787	−1.253722
73	6	0	7.159359	2.826003	−1.900014
74	6	0	6.358504	2.198803	−2.942733
75	6	0	5.057430	2.812764	−2.938756
76	6	0	5.991909	−2.344999	1.118912
77	6	0	5.881694	−2.570940	−0.307651
78	6	0	6.989255	−1.886594	−0.941535
79	6	0	7.797045	−1.262372	0.097261
80	6	0	7.182546	−1.545034	1.366326
81	6	0	4.849146	−2.147843	1.883052

82	6	0	4.832951	−1.147633	2.934711
83	6	0	3.531428	−0.533882	2.938645
84	6	0	2.729347	−1.161882	1.897277
85	6	0	3.541810	−2.169735	1.250330
86	6	0	2.708019	3.210266	−1.370570
87	6	0	2.093277	2.927253	−0.100396
88	6	0	2.900086	3.551628	0.938358
89	6	0	4.008312	4.235183	0.304220
90	6	0	3.898159	4.009462	−1.123031
91	6	0	5.306001	0.023534	−3.423963
92	6	0	6.496010	0.828956	−3.181514
93	6	0	7.422935	0.042554	−2.411748
94	6	0	6.808099	−1.247465	−2.161561
95	6	0	5.503660	−1.268026	−2.801432
96	6	0	1.532170	0.671156	−0.906784
97	6	0	1.725342	−0.622152	−0.279458
98	6	0	1.836130	−0.401705	1.152596
99	6	0	1.692592	1.019551	1.405562
100	6	0	1.508949	1.680489	0.140045
101	6	0	3.393861	0.835360	3.178303
102	6	0	4.583839	1.640262	3.419831
103	6	0	4.385842	2.932267	2.797044
104	6	0	3.080837	2.912486	2.158360
105	6	0	2.466361	1.622133	2.408089
106	6	0	8.166459	2.287924	0.276649
107	6	0	8.362017	0.994870	0.903462
108	6	0	8.382943	−0.014772	−0.143805
109	6	0	8.196900	0.645287	−1.408048
110	6	0	8.051813	2.065906	−1.154803
111	6	0	5.452383	3.586633	2.186208
112	6	0	6.764976	2.969186	2.178258
113	6	0	7.385221	3.254059	0.897877
114	6	0	6.454138	4.047261	0.118692
115	6	0	5.262672	4.251893	0.914523
116	6	0	7.162898	−0.576458	2.376312
117	6	0	7.768693	0.721542	2.127901
118	6	0	6.954593	1.730871	2.778595
119	6	0	5.840046	1.048487	3.412762
120	6	0	5.979714	−0.374787	3.169116

C_{60}^- (doublet) by UM06-2x/6-31G(d)/SMD(oDCB)

E(UM062X) = −2285.63286005 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2285.301876 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.350901	3.320571	1.182150
2	6	0	−1.692857	3.012166	0.726393
3	6	0	−1.694774	3.024199	−0.726698
4	6	0	0.476354	3.498272	0.004770
5	6	0	−0.360964	3.322279	−1.170640
6	6	0	0.165804	2.695247	2.311440
7	6	0	1.536564	2.222436	2.311687
8	6	0	1.574747	0.967437	3.036037
9	6	0	−0.640355	1.733611	3.036721
10	6	0	0.230660	0.666182	3.483704
11	6	0	−2.464984	2.092407	1.421476
12	6	0	−1.928845	1.440578	2.600060
13	6	0	−2.401166	0.068739	2.589068
14	6	0	−3.281551	1.129023	0.699751
15	6	0	−3.244924	−0.114496	1.419232
16	6	0	−2.480424	2.094199	−1.419772
17	6	0	−3.278029	1.139457	−0.700000
18	6	0	−3.231774	−0.122736	−1.421254
19	6	0	−1.929941	1.428923	−2.589108
20	6	0	−2.407393	0.058895	−2.600231
21	6	0	1.787587	3.044662	0.004828
22	6	0	2.339651	2.391860	−1.171353
23	6	0	3.204436	1.332611	−0.726928
24	6	0	2.330673	2.396857	1.182979
25	6	0	3.195604	1.324407	0.726935
26	6	0	0.169868	2.688250	−2.300742
27	6	0	−0.641800	1.717800	−3.018580
28	6	0	0.225150	0.649800	−3.476171
29	6	0	1.529100	2.219409	−2.300951
30	6	0	1.566276	0.954034	−3.017752
31	6	0	0.350901	−3.320571	−1.182150
32	6	0	−0.476354	−3.498272	−0.004770
33	6	0	0.360964	−3.322279	1.170640
34	6	0	1.692857	−3.012166	−0.726393
35	6	0	1.694774	−3.024199	0.726698
36	6	0	−0.165804	−2.695247	−2.311440
37	6	0	0.640355	−1.733611	−3.036721
38	6	0	−0.230660	−0.666182	−3.483704
39	6	0	−1.536564	−2.222436	−2.311687
40	6	0	−1.574747	−0.967437	−3.036037
41	6	0	−1.787587	−3.044662	−0.004828
42	6	0	−2.330673	−2.396857	−1.182979
43	6	0	−3.195604	−1.324407	−0.726935
44	6	0	−2.339651	−2.391860	1.171353
45	6	0	−3.204436	−1.332611	0.726928
46	6	0	−0.169868	−2.688250	2.300742
47	6	0	−1.529100	−2.219409	2.300951
48	6	0	−1.566276	−0.954034	3.017752
49	6	0	0.641800	−1.717800	3.018580
50	6	0	−0.225150	−0.649800	3.476171
51	6	0	2.464984	−2.092407	−1.421476
52	6	0	3.281551	−1.129023	−0.699751
53	6	0	3.244924	0.114496	−1.419232
54	6	0	1.928845	−1.440578	−2.600060
55	6	0	2.401166	−0.068739	−2.589068
56	6	0	2.480424	−2.094199	1.419772
57	6	0	1.929941	−1.428923	2.589108
58	6	0	2.407393	−0.058895	2.600231
59	6	0	3.278029	−1.139457	0.700000
60	6	0	3.231774	0.122736	1.421254

C_{60}^- dimer (singlet) by M06-2x/6-31G(d)/SMD(oDCB)

E(RM062X) = −4571.27423907 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4570.579121 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−7.891878	−0.762033	−1.174150
2	6	0	−7.424788	−2.062367	−0.726449
3	6	0	−7.424706	−2.062529	0.726259
4	6	0	−7.891776	−0.762302	1.174316
5	6	0	−8.174555	0.040645	0.000192
6	6	0	−5.783002	1.442266	3.015090
7	6	0	−7.025545	1.248234	2.297616
8	6	0	−7.319456	−0.175760	2.296137
9	6	0	−6.274105	−0.858787	3.030992
10	6	0	−5.314414	0.138919	3.459362
11	6	0	−5.814769	−2.098282	−2.591924
12	6	0	−4.408750	−2.420097	−2.603656
13	6	0	−4.124901	−3.204639	−1.423245
14	6	0	−5.365986	−3.404676	−0.694147
15	6	0	−6.416391	−2.715658	−1.419641
16	6	0	−3.009876	0.851919	3.000336
17	6	0	−3.954575	−0.145212	3.444466
18	6	0	−3.473776	−1.450418	3.000124
19	6	0	−2.228538	−1.272858	2.320866
20	6	0	−1.954662	0.171578	2.281808
21	6	0	−3.455853	2.106883	2.587278
22	6	0	−2.871802	2.717580	1.424643
23	6	0	−3.928424	3.404135	0.692744
24	6	0	−5.168729	3.207342	1.417411
25	6	0	−4.874120	2.404076	2.591443
26	6	0	−7.319697	−0.175227	−2.295904
27	6	0	−7.025769	1.248754	−2.297081
28	6	0	−5.783310	1.442960	−3.014640
29	6	0	−5.314754	0.139732	−3.459248
30	6	0	−6.274399	−0.858088	−3.031001
31	6	0	−6.416229	−2.715975	1.419188
32	6	0	−5.365909	−3.404824	0.693420
33	6	0	−4.124744	−3.204943	1.422430
34	6	0	−4.408484	−2.420700	2.603099
35	6	0	−5.814472	−2.098862	2.591549
36	6	0	−7.900112	1.404003	0.000331
37	6	0	−7.307465	2.016488	1.173719
38	6	0	−6.359093	3.019075	0.726007
39	6	0	−6.359170	3.019242	−0.725138
40	6	0	−7.307572	2.016748	−1.172975
41	6	0	−3.928500	3.404310	−0.692035
42	6	0	−2.871953	2.717894	−1.424191
43	6	0	−3.456112	2.107470	−2.586900
44	6	0	−4.874377	2.404680	−2.590864
45	6	0	−5.168867	3.207680	−1.416617

46	6	0	−1.979382	−1.995358	−1.142119
47	6	0	−1.347913	−1.440559	−0.000310
48	6	0	−1.979241	−1.995596	1.141365
49	6	0	−2.944376	−3.012226	0.717964
50	6	0	−2.944464	−3.012054	−0.718848
51	6	0	−3.010167	0.852611	−3.000301
52	6	0	−1.954885	0.172120	−2.282018
53	6	0	−2.228860	−1.272300	−2.321292
54	6	0	−3.474115	−1.449735	−3.000582
55	6	0	−3.954922	−0.144414	−3.444571
56	6	0	−1.379105	0.763977	1.177832
57	6	0	−0.789323	−0.029236	−0.000187
58	6	0	−1.379208	0.764250	−1.177972
59	6	0	−1.879149	2.031190	−0.726907
60	6	0	−1.879085	2.031007	0.727112
61	6	0	1.979243	1.995427	1.141660
62	6	0	2.944376	3.012120	0.718406
63	6	0	2.944461	3.012159	−0.718406
64	6	0	1.979379	1.995525	−1.141824
65	6	0	1.347912	1.440557	−0.000097
66	6	0	3.010162	−0.852170	−3.000429
67	6	0	1.954881	−0.171785	−2.282045
68	6	0	2.228854	1.272641	−2.321106
69	6	0	3.474107	1.450176	−3.000372
70	6	0	3.954914	0.144921	−3.444553
71	6	0	4.408489	2.420316	2.603448
72	6	0	5.814478	2.098480	2.591848
73	6	0	6.416233	2.715768	1.419577
74	6	0	5.365909	3.404722	0.693914
75	6	0	4.124747	3.204733	1.422897
76	6	0	5.783303	−1.442516	−3.014862
77	6	0	5.314746	−0.139222	−3.459278
78	6	0	6.274392	0.858534	−3.030886
79	6	0	7.319692	0.175566	−2.295890
80	6	0	7.025766	−1.248416	−2.297278
81	6	0	4.874372	−2.404297	−2.591224
82	6	0	5.168866	−3.207469	−1.417096
83	6	0	3.928500	−3.404208	−0.692540
84	6	0	2.871949	−2.717687	−1.424593
85	6	0	3.456107	−2.107089	−2.587213
86	6	0	2.228543	1.272515	2.321052
87	6	0	1.954667	−0.171916	2.281782
88	6	0	3.009882	−0.852361	3.000209
89	6	0	3.954582	0.144704	3.444483
90	6	0	3.473784	1.449975	3.000334
91	6	0	4.124896	3.204849	−1.422779
92	6	0	5.365982	3.404779	−0.693654
93	6	0	6.416384	2.715867	−1.419251
94	6	0	5.814761	2.098664	−2.591625
95	6	0	4.408742	2.420481	−2.603307
96	6	0	0.789323	0.029234	−0.000182
97	6	0	1.379208	−0.764077	−1.178084
98	6	0	1.879147	−2.031084	−0.727206
99	6	0	1.879089	−2.031116	0.726813
100	6	0	1.379105	−0.764153	1.177720
101	6	0	3.928427	−3.404238	0.692239
102	6	0	5.168733	−3.207552	1.416931
103	6	0	4.874127	−2.404458	2.591083
104	6	0	3.455859	−2.107264	2.586965
105	6	0	2.871808	−2.717790	1.424241
106	6	0	7.891778	0.762130	1.174414
107	6	0	8.174555	−0.040644	0.000171
108	6	0	7.891875	0.762208	−1.174052
109	6	0	7.424784	2.062474	−0.726159
110	6	0	7.424708	2.062424	0.726549
111	6	0	5.783010	−1.442709	3.014868
112	6	0	7.025550	−1.248571	2.297419
113	6	0	7.319461	0.175423	2.296151
114	6	0	6.274110	0.858342	3.031107
115	6	0	5.314422	−0.139429	3.459333
116	6	0	7.307572	−2.016575	−1.173286
117	6	0	7.900113	−1.404002	0.000109
118	6	0	7.307467	−2.016659	1.173408
119	6	0	6.359096	−3.019181	0.725552
120	6	0	6.359170	−3.019134	−0.725592

C_{60}^- dimer (triplet) by UM06-2x/6-31G(d)/SMD(oDCB)

E(UM062X) = −4571.26418153 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4570.583027 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−8.419182	0.019716	−0.217375
2	6	0	−8.226668	−0.724339	−1.432040
3	6	0	−8.107112	−2.129633	−1.085574
4	6	0	−8.237207	−2.254173	0.355322
5	6	0	−8.417890	−0.917814	0.892630
6	6	0	−5.557506	−3.460099	2.369571
7	6	0	−6.859569	−2.828136	2.310139
8	6	0	−7.474517	−3.187448	1.046470
9	6	0	−6.548407	−4.041155	0.327550
10	6	0	−5.365771	−4.209363	1.146879
11	6	0	−6.804206	1.094596	−2.295592
12	6	0	−5.497900	1.054547	−2.925652
13	6	0	−5.314788	−0.279210	−3.457482
14	6	0	−6.518003	−1.050817	−3.177016
15	6	0	−7.435889	−0.203061	−2.465170
16	6	0	−2.993313	−3.542620	1.143812
17	6	0	−4.108779	−4.250529	0.546284
18	6	0	−3.983931	−4.122941	−0.889936
19	6	0	−2.780391	−3.356888	−1.177175
20	6	0	−2.167381	−3.003525	0.075794
21	6	0	−3.177632	−2.823528	2.316998
22	6	0	−2.546580	−1.525767	2.486236
23	6	0	−3.464812	−0.677575	3.198345
24	6	0	−4.667861	−1.448852	3.478269
25	6	0	−4.484455	−2.782972	2.946213
26	6	0	−7.815588	1.274750	−0.054331
27	6	0	−7.202453	1.627687	1.197717
28	6	0	−5.998549	2.394359	0.910569
29	6	0	−5.873646	2.522129	−0.525069
30	6	0	−6.988658	1.813560	−1.122275
31	6	0	−7.221417	−2.948161	−1.772739
32	6	0	−6.403368	−2.405145	−2.847690
33	6	0	−5.111575	−3.034642	−2.790833
34	6	0	−5.116793	−3.962825	−1.676248
35	6	0	−6.427914	−3.922724	−1.052552
36	6	0	−7.828388	−0.574629	2.101635
37	6	0	−7.035915	−1.548358	2.825054
38	6	0	−5.915670	−0.841701	3.422913
39	6	0	−6.031709	0.565149	3.085981
40	6	0	−7.204447	0.729426	2.269457
41	6	0	−3.579332	0.676092	2.868251
42	6	0	−2.760155	1.220003	1.794508
43	6	0	−3.553995	2.193623	1.073889
44	6	0	−4.865702	2.233287	1.696821
45	6	0	−4.871289	1.305777	2.811693
46	6	0	−2.946526	−0.180563	−2.803820
47	6	0	−2.153766	−1.154537	−2.080978
48	6	0	−2.778738	−2.458197	−2.247745
49	6	0	−3.951393	−2.293802	−3.064862
50	6	0	−4.067153	−0.886864	−3.401404
51	6	0	−3.433564	2.311780	−0.306135
52	6	0	−2.506904	1.458586	−1.025054
53	6	0	−3.122469	1.098903	−2.288717
54	6	0	−4.424353	1.731052	−2.347894
55	6	0	−4.615977	2.480088	−1.125628
56	6	0	−1.564988	−1.749368	0.238312
57	6	0	−1.566549	−0.811847	−0.871439
58	6	0	−1.745824	0.524797	−0.333696
59	6	0	−1.873852	0.401303	1.107804
60	6	0	−1.756456	−1.004410	1.453918
61	6	0	2.783310	2.459839	−2.254231
62	6	0	3.957333	2.294597	−3.068892
63	6	0	4.072783	0.887242	−3.405696
64	6	0	2.950876	0.181772	−2.810225
65	6	0	2.157926	1.156339	−2.088295
66	6	0	3.432299	−2.311197	−0.311976
67	6	0	2.507502	−1.457484	−1.032387
68	6	0	3.125070	−1.098102	−2.294947
69	6	0	4.426714	−1.730692	−2.352282
70	6	0	4.616136	−2.480045	−1.129515
71	6	0	5.121329	3.963041	−1.678614
72	6	0	6.431267	3.922125	−1.053130
73	6	0	7.225153	2.946791	−1.772322
74	6	0	6.409009	2.404695	−2.848877
75	6	0	5.117466	3.034457	−2.793398
76	6	0	5.995493	−2.395410	0.908829
77	6	0	5.872543	−2.522866	−0.527312
78	6	0	6.989162	−1.815135	−1.122742
79	6	0	7.814520	−1.277030	−0.053312

80	6	0	7.199356	−1.629691	1.197666
81	6	0	4.861416	−2.233750	1.692939
82	6	0	4.865660	−1.305845	2.808022
83	6	0	3.573968	−0.675885	2.863179
84	6	0	2.756651	−1.218887	1.787839
85	6	0	3.550883	−2.193278	1.068226
86	6	0	2.783770	3.358620	−1.183384
87	6	0	2.168738	3.005495	0.068521
88	6	0	2.993053	3.543936	1.138036
89	6	0	4.110111	4.251015	0.542290
90	6	0	3.987231	4.123740	−0.894438
91	6	0	5.320182	0.279292	−3.460061
92	6	0	6.523378	1.049951	−3.178291
93	6	0	7.439200	0.201681	−2.464699
94	6	0	6.806802	−1.096044	−2.296252
95	6	0	5.501568	−1.055024	−2.928038
96	6	0	1.568657	0.813843	−0.879687
97	6	0	1.746051	−0.522984	−0.341922
98	6	0	1.871999	−0.399724	1.099616
99	6	0	1.754810	1.006307	1.445820
100	6	0	1.565527	1.751450	0.230065
101	6	0	3.459706	0.678179	3.193359
102	6	0	4.662727	1.448500	3.474594
103	6	0	4.481034	2.783181	2.942355
104	6	0	3.175276	2.824702	2.311409
105	6	0	2.543489	1.526892	2.479515
106	6	0	8.237335	2.252140	0.357272
107	6	0	8.416103	0.915573	0.894587
108	6	0	8.418902	−0.022070	−0.215417
109	6	0	8.228488	0.722174	−1.430162
110	6	0	8.109174	2.127804	−1.083613
111	6	0	5.555386	3.459465	2.367702
112	6	0	6.857249	2.827081	2.310104
113	6	0	7.474169	3.186086	1.047555
114	6	0	6.549913	4.040291	0.327153
115	6	0	5.365848	4.209060	1.144532
116	6	0	7.200178	−0.731328	2.269684
117	6	0	7.824537	0.572575	2.102683
118	6	0	7.031852	1.546881	2.825179
119	6	0	5.910316	0.841058	3.420931
120	6	0	6.026040	−0.566187	3.083726

C_{60}^- (doublet) by UωB97XD/6-31G(d) without solvent parameters

E(UwB97XD) = −2285.51972287 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2285.193751 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−1.357313	3.041316	1.188633
2	6	0	−2.537989	2.318308	0.726669
3	6	0	−2.549989	2.348308	−0.729669
4	6	0	−0.637453	3.462539	0.010500
5	6	0	−1.387313	3.041316	−1.164633
6	6	0	−0.686422	2.608989	2.317152
7	6	0	0.771178	2.585500	2.317328
8	6	0	1.197931	1.419146	3.047690
9	6	0	−1.151508	1.457474	3.047500
10	6	0	0.011199	0.712025	3.485675
11	6	0	−2.976347	1.218014	1.419084
12	6	0	−2.280586	0.773753	2.610421
13	6	0	−2.296711	−0.671987	2.583443
14	6	0	−3.474813	0.040173	0.702241
15	6	0	−3.056287	−1.110759	1.416064
16	6	0	−3.018347	1.209014	−1.416084
17	6	0	−3.474813	0.073173	−0.702241
18	6	0	−3.014287	−1.119759	−1.419064
19	6	0	−2.274586	0.746753	−2.583421
20	6	0	−2.305711	−0.698987	−2.610443
21	6	0	0.749913	3.439997	0.010500
22	6	0	1.485712	2.995070	−1.164761
23	6	0	2.626026	2.264287	−0.729665
24	6	0	1.455712	2.995070	1.188761
25	6	0	2.611026	2.234287	0.726665
26	6	0	−0.668422	2.602989	−2.299152
27	6	0	−1.142508	1.421474	−3.005500
28	6	0	0.011199	0.673025	−3.470675
29	6	0	0.753178	2.579500	−2.299328
30	6	0	1.188931	1.383146	−3.005690
31	6	0	1.357313	−3.041316	−1.188633
32	6	0	0.637453	−3.462539	−0.010500
33	6	0	1.387313	−3.041316	1.164633
34	6	0	2.537989	−2.318308	−0.726669
35	6	0	2.549989	−2.348308	0.729669
36	6	0	0.686422	−2.608989	−2.317152
37	6	0	1.151508	−1.457474	−3.047500
38	6	0	−0.011199	−0.712025	−3.485675
39	6	0	−0.771178	−2.585500	−2.317328
40	6	0	−1.197931	−1.419146	−3.047690
41	6	0	−0.749913	−3.439997	−0.010500
42	6	0	−1.455712	−2.995070	−1.188761
43	6	0	−2.611026	−2.234287	−0.726665
44	6	0	−1.485712	−2.995070	1.164761
45	6	0	−2.626026	−2.264287	0.729665
46	6	0	0.668422	−2.602989	2.299152
47	6	0	−0.753178	−2.579500	2.299328
48	6	0	−1.188931	−1.383146	3.005690
49	6	0	1.142508	−1.421474	3.005500
50	6	0	−0.011199	−0.673025	3.470675
51	6	0	2.976347	−1.218014	−1.419084
52	6	0	3.474813	−0.040173	−0.702241
53	6	0	3.056287	1.110759	−1.416064
54	6	0	2.280586	−0.773753	−2.610421
55	6	0	2.296711	0.671987	−2.583443
56	6	0	3.018347	−1.209014	1.416084
57	6	0	2.274586	−0.746753	2.583421
58	6	0	2.305711	0.698987	2.610443
59	6	0	3.474813	−0.073173	0.702241
60	6	0	3.014287	1.119759	1.419064

C_{60}^- dimer (singlet) by ωB97XD/6-31G(d) without solvent parameters

E(RwB97XD) = −4571.03347492 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4570.334927 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−7.888301	−0.761735	−1.173370
2	6	0	−7.421014	−2.060401	−0.725736
3	6	0	−7.421015	−2.060452	0.725591
4	6	0	−7.888304	−0.761819	1.173314
5	6	0	−8.169446	0.040175	0.000000
6	6	0	−5.779892	1.440959	3.012376
7	6	0	−7.020813	1.247005	2.294739
8	6	0	−7.314328	−0.175334	2.293085
9	6	0	−6.271126	−0.857811	3.029424
10	6	0	−5.311844	0.139206	3.456459
11	6	0	−5.810603	−2.095645	−2.588847
12	6	0	−4.406521	−2.419728	−2.602812
13	6	0	−4.123689	−3.201704	−1.422162
14	6	0	−5.362896	−3.400954	−0.693523
15	6	0	−6.412311	−2.712458	−1.417558
16	6	0	−3.008825	0.851434	2.995544
17	6	0	−3.953424	−0.144250	3.439020
18	6	0	−3.473064	−1.447428	2.994918
19	6	0	−2.228786	−1.270614	2.318487
20	6	0	−1.956065	0.172055	2.277765
21	6	0	−3.453700	2.106059	2.584944
22	6	0	−2.870452	2.715851	1.423445
23	6	0	−3.926544	3.399871	0.691993
24	6	0	−5.165684	3.203051	1.415065
25	6	0	−4.871291	2.401190	2.588249
26	6	0	−7.314322	−0.175172	−2.293098
27	6	0	−7.020807	1.247166	−2.294650
28	6	0	−5.779884	1.441171	−3.012270
29	6	0	−5.311834	0.139448	−3.456443
30	6	0	−6.271118	−0.857598	−3.029482
31	6	0	−6.412314	−2.712557	1.417370
32	6	0	−5.362898	−3.401004	0.693290
33	6	0	−4.123693	−3.201806	1.421945
34	6	0	−4.406528	−2.419912	2.602650
35	6	0	−5.810610	−2.095827	2.588704
36	6	0	−7.896115	1.402777	0.000049
37	6	0	−7.303077	2.014782	1.171889
38	6	0	−6.356365	3.017222	0.724808
39	6	0	−6.356363	3.017272	−0.724592
40	6	0	−7.303074	2.014863	−1.171746
41	6	0	−3.926542	3.399921	−0.691745
42	6	0	−2.870449	2.715951	−1.423242
43	6	0	−3.453693	2.106241	−2.584786

44	6	0	−4.871284	2.401373	−2.588074
45	6	0	−5.165680	3.203152	−1.414833
46	6	0	−1.982775	−1.990873	−1.139085
47	6	0	−1.349172	−1.439310	−0.000043
48	6	0	−1.982781	−1.990953	1.138958
49	6	0	−2.945278	−3.007591	0.717300
50	6	0	−2.945275	−3.007541	−0.717501
51	6	0	−3.008817	0.851644	−2.995472
52	6	0	−1.956059	0.172217	−2.277737
53	6	0	−2.228779	−1.270449	−2.318562
54	6	0	−3.473055	−1.447217	−2.995009
55	6	0	−3.953414	−0.144009	−3.439021
56	6	0	−1.381451	0.764003	1.175934
57	6	0	−0.787908	−0.028419	0.000008
58	6	0	−1.381449	0.764087	−1.175862
59	6	0	−1.881075	2.027802	−0.725617
60	6	0	−1.881077	2.027750	0.725776
61	6	0	1.982781	1.990785	1.139249
62	6	0	2.945279	3.007486	0.717739
63	6	0	2.945275	3.007646	−0.717062
64	6	0	1.982776	1.991041	−1.138794
65	6	0	1.349172	1.439310	0.000167
66	6	0	3.008812	−0.851204	−2.995602
67	6	0	1.956055	−0.171881	−2.277766
68	6	0	2.228776	1.270791	−2.318378
69	6	0	3.473051	1.447658	−2.994802
70	6	0	3.953408	0.144514	−3.439006
71	6	0	4.406533	2.419528	2.602999
72	6	0	5.810614	2.095446	2.589002
73	6	0	6.412317	2.712349	1.417758
74	6	0	5.362899	3.400901	0.693781
75	6	0	4.123695	3.201595	1.422409
76	6	0	5.779879	−1.440728	−3.012492
77	6	0	5.311828	−0.138940	−3.456473
78	6	0	6.271113	0.858044	−3.029366
79	6	0	7.314318	0.175510	−2.293083
80	6	0	7.020803	−1.246829	−2.294846
81	6	0	4.871279	−2.400992	−2.588435
82	6	0	5.165677	−3.202943	−1.415313
83	6	0	3.926541	−3.399819	−0.692252
84	6	0	2.870446	−2.715742	−1.423646
85	6	0	3.453689	−2.105860	−2.585101
86	6	0	2.228789	1.270271	2.318671
87	6	0	1.956069	−0.172392	2.277736
88	6	0	3.008830	−0.851875	2.995414
89	6	0	3.953429	0.143744	3.439035
90	6	0	3.473068	1.446987	2.995125
91	6	0	4.123686	3.201915	−1.421697
92	6	0	5.362895	3.401057	−0.693032
93	6	0	6.412308	2.712666	−1.417170
94	6	0	5.810598	2.096026	−2.588549
95	6	0	4.406517	2.420112	−2.602463
96	6	0	0.787908	0.028419	0.000011
97	6	0	1.381447	−0.763913	−1.175978
98	6	0	1.881074	−2.027694	−0.725919
99	6	0	1.881079	−2.027857	0.725473
100	6	0	1.381454	−0.764177	1.175818
101	6	0	3.926545	−3.399974	0.691487
102	6	0	5.165686	−3.203260	1.414585
103	6	0	4.871296	−2.401572	2.587888
104	6	0	3.453705	−2.106440	2.584629
105	6	0	2.870455	−2.716060	1.423041
106	6	0	7.888306	0.761645	1.173414
107	6	0	8.169446	−0.040175	−0.000019
108	6	0	7.888299	0.761909	−1.173270
109	6	0	7.421012	2.060508	−0.725446
110	6	0	7.421017	2.060345	0.725882
111	6	0	5.779897	−1.441402	3.012154
112	6	0	7.020817	−1.247343	2.294543
113	6	0	7.314332	0.174996	2.293099
114	6	0	6.271131	0.857365	3.029540
115	6	0	5.311849	−0.139714	3.456429
116	6	0	7.303072	−2.014691	−1.172055
117	6	0	7.896115	−1.402777	−0.000171
118	6	0	7.303079	−2.014953	1.171579
119	6	0	6.356366	−3.017328	0.724353
120	6	0	6.356362	−3.017166	−0.725047

C_{60}^- dimer (triplet) by UωB97XD/6-31G(d) without solvent parameters

E(UwB97XD) = −4571.01820173 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4570.336751 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.284631	1.423942	0.065771
2	6	0	8.202389	0.818770	1.376665
3	6	0	8.309854	−0.614692	1.216100
4	6	0	8.459771	−0.897735	−0.196609
5	6	0	8.443561	0.364310	−0.908723
6	6	0	5.996030	−2.751237	−1.999022
7	6	0	7.183565	−1.916034	−2.036699
8	6	0	7.843991	−2.012493	−0.750394
9	6	0	7.046935	−2.893827	0.081674
10	6	0	5.914227	−3.354267	−0.697745
11	6	0	6.513045	2.494623	2.009403
12	6	0	5.224189	2.331117	2.659925
13	6	0	5.239996	1.080088	3.366328
14	6	0	6.538767	0.463071	3.157152
15	6	0	7.334304	1.346088	2.330477
16	6	0	3.467774	−3.066702	−0.746992
17	6	0	4.670679	−3.516324	−0.071525
18	6	0	4.522206	−3.232471	1.328658
19	6	0	3.221324	−2.613690	1.529665
20	6	0	2.561977	−2.522224	0.245188
21	6	0	3.546287	−2.485931	−2.004178
22	6	0	2.725217	−1.337976	−2.325740
23	6	0	3.520559	−0.454787	−3.151652
24	6	0	4.820555	−1.071122	−3.359776
25	6	0	4.836361	−2.321730	−2.653579
26	6	0	7.498138	2.530343	−0.240462
27	6	0	6.838269	2.622045	−1.525023
28	6	0	5.538464	3.242359	−1.324356
29	6	0	5.390039	3.525854	0.076266
30	6	0	6.591927	3.075706	0.751776
31	6	0	7.548235	−1.462649	2.013654
32	6	0	6.642097	−0.912395	3.003907
33	6	0	5.456536	−1.746196	3.052414
34	6	0	5.614413	−2.795379	2.083400
35	6	0	6.904347	−2.622402	1.434846
36	6	0	7.812335	0.454695	−2.142532
37	6	0	7.168036	−0.708258	−2.718164
38	6	0	5.964550	−0.266762	−3.401316
39	6	0	5.857540	1.157334	−3.244416
40	6	0	6.990109	1.607257	−2.458972
41	6	0	3.417378	0.920093	−2.998227
42	6	0	2.511244	1.470877	−2.009033
43	6	0	3.154934	2.629978	−1.429900
44	6	0	4.446263	2.801899	−2.077141
45	6	0	4.604156	1.753433	−3.046228
46	6	0	2.891920	0.716530	2.722209
47	6	0	2.248076	−0.446589	2.147356
48	6	0	3.070102	−1.598859	2.462644
49	6	0	4.203490	−1.148707	3.247578
50	6	0	4.096454	0.275154	3.404258
51	6	0	3.012996	2.900807	−0.077177
52	6	0	2.216321	2.020666	0.755067
53	6	0	2.876266	1.923562	2.041134
54	6	0	4.064986	2.757652	2.002898
55	6	0	4.146789	3.360697	0.702029
56	6	0	1.778768	−1.415062	−0.060926
57	6	0	1.623273	−0.355733	0.912626
58	6	0	1.605570	0.905284	0.201061
59	6	0	1.751920	0.622643	−1.210950
60	6	0	1.859288	−0.810315	−1.371369
61	6	0	−3.061799	1.606017	2.446747
62	6	0	−4.192956	1.158817	3.236509
63	6	0	−4.086036	−0.264543	3.397588
64	6	0	−2.883851	−0.708670	2.713340
65	6	0	−2.241289	0.452322	2.132588
66	6	0	−3.014658	−2.902057	−0.078603
67	6	0	−2.215001	−2.019480	0.748345
68	6	0	−2.870766	−1.917858	2.036099
69	6	0	−4.060140	−2.751490	2.003999
70	6	0	−4.146117	−3.359007	0.705448
71	6	0	−5.606750	2.802173	2.071090
72	6	0	−6.898861	2.627650	1.427066
73	6	0	−7.541439	1.470203	2.011627
74	6	0	−6.632448	0.922733	3.000771
75	6	0	−5.446355	1.756162	3.043101
76	6	0	−5.544052	−3.246489	−1.317020
77	6	0	−5.391498	−3.525725	0.084079

78	6	0	−6.590942	−3.072790	0.761678
79	6	0	−7.500016	−2.530150	−0.229628
80	6	0	−6.844282	−2.626444	−1.515950
81	6	0	−4.454054	−2.808960	−2.074481
82	6	0	−4.614474	−1.763607	−3.046584
83	6	0	−3.427156	−0.930666	−3.004791
84	6	0	−2.518185	−1.478680	−2.016684
85	6	0	−3.160560	−2.635499	−1.431800
86	6	0	−3.215435	2.617833	1.510910
87	6	0	−2.560206	2.521793	0.224681
88	6	0	−3.468887	3.063509	−0.766545
89	6	0	−4.669344	3.515950	−0.088956
90	6	0	−4.516737	3.236385	1.311663
91	6	0	−5.230121	−1.069091	3.365688
92	6	0	−6.529189	−0.452273	3.158229
93	6	0	−7.327739	−1.337674	2.336964
94	6	0	−6.508085	−2.487507	2.017124
95	6	0	−5.216998	−2.322309	2.663090
96	6	0	−1.620400	0.357086	0.896331
97	6	0	−1.605332	−0.906294	0.188727
98	6	0	−1.755969	−0.628091	−1.223656
99	6	0	−1.863233	0.804273	−1.388447
100	6	0	−1.778594	1.413315	−0.080276
101	6	0	−3.530266	0.443751	−3.162429
102	6	0	−4.830558	1.059894	−3.368795
103	6	0	−4.843667	2.312726	−2.666418
104	6	0	−3.551374	2.478596	−2.021579
105	6	0	−2.731930	1.329318	−2.341896
106	6	0	−8.459988	0.898451	−0.193944
107	6	0	−8.446494	−0.365937	−0.902128
108	6	0	−8.284964	−1.422477	0.075436
109	6	0	−8.198608	−0.812972	1.384073
110	6	0	−8.305967	0.619856	1.219133
111	6	0	−6.000980	2.744819	−2.009763
112	6	0	−7.189173	1.910071	−2.041343
113	6	0	−7.845449	2.011077	−0.753364
114	6	0	−7.045399	2.894842	0.073418
115	6	0	−5.915049	3.352373	−0.710827
116	6	0	−6.998547	−1.614696	−2.452790
117	6	0	−7.819260	−0.460701	−2.137497
118	6	0	−7.176218	0.700164	−2.719022
119	6	0	−5.975098	0.255941	−3.404341
120	6	0	−5.868179	−1.167703	−3.242998

C_{60}^- (doublet) by UωB97XD/6-31G(d)/SMD(oDCB)

E(UwB97XD) = −2285.62373002 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −2285.291876 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.350638	3.317455	1.180892
2	6	0	−1.691329	3.009502	0.725800
3	6	0	−1.693177	3.021444	−0.725600
4	6	0	0.475484	3.494350	0.004982
5	6	0	−0.360389	3.318785	−1.168914
6	6	0	0.165783	2.692149	2.308899
7	6	0	1.534544	2.219416	2.309053
8	6	0	1.572958	0.966287	3.032765
9	6	0	−0.639561	1.731656	3.033115
10	6	0	0.230330	0.665550	3.480046
11	6	0	−2.462492	2.090207	1.420144
12	6	0	−1.927067	1.439225	2.597217
13	6	0	−2.398309	0.069002	2.586105
14	6	0	−3.278025	1.128116	0.699375
15	6	0	−3.240897	−0.114216	1.418006
16	6	0	−2.477749	2.091585	−1.418550
17	6	0	−3.274622	1.137935	−0.699555
18	6	0	−3.227996	−0.122616	−1.419925
19	6	0	−1.928054	1.427300	−2.586201
20	6	0	−2.404967	0.059044	−2.597501
21	6	0	1.785781	3.041631	0.005016
22	6	0	2.336518	2.388921	−1.169387
23	6	0	3.200546	1.331067	−0.725634
24	6	0	2.327966	2.393965	1.181495
25	6	0	3.191815	1.322904	0.726172
26	6	0	0.169653	2.684861	−2.298401
27	6	0	−0.641142	1.715766	−3.015218
28	6	0	0.224825	0.649243	−3.472883
29	6	0	1.527121	2.216071	−2.298500
30	6	0	1.564520	0.952835	−3.014711
31	6	0	0.350638	−3.317455	−1.180892
32	6	0	−0.475484	−3.494350	−0.004982
33	6	0	0.360389	−3.318785	1.168914
34	6	0	1.691329	−3.009502	−0.725800
35	6	0	1.693177	−3.021444	0.725600
36	6	0	−0.165783	−2.692149	−2.308899
37	6	0	0.639561	−1.731656	−3.033115
38	6	0	−0.230330	−0.665550	−3.480046
39	6	0	−1.534544	−2.219416	−2.309053
40	6	0	−1.572958	−0.966287	−3.032765
41	6	0	−1.785781	−3.041631	−0.005016
42	6	0	−2.327966	−2.393965	−1.181495
43	6	0	−3.191815	−1.322904	−0.726172
44	6	0	−2.336518	−2.388921	1.169387
45	6	0	−3.200546	−1.331067	0.725634
46	6	0	−0.169653	−2.684861	2.298401
47	6	0	−1.527121	−2.216071	2.298500
48	6	0	−1.564520	−0.952835	3.014711
49	6	0	0.641142	−1.715766	3.015218
50	6	0	−0.224825	−0.649243	3.472883
51	6	0	2.462492	−2.090207	−1.420144
52	6	0	3.278025	−1.128116	−0.699375
53	6	0	3.240897	0.114216	−1.418006
54	6	0	1.927067	−1.439225	−2.597217
55	6	0	2.398309	−0.069002	−2.586105
56	6	0	2.477749	−2.091585	1.418550
57	6	0	1.928054	−1.427300	2.586201
58	6	0	2.404967	−0.059044	2.597501
59	6	0	3.274622	−1.137935	0.699555
60	6	0	3.227996	0.122616	1.419925

C_{60}^- dimer (singlet) by ωB97XD/6-31G(d)/SMD(oDCB)

E(RwB97XD) = −4571.27172954 au (*C*1 symmetry)

Sum of electronic and thermal Free Energies= −4570.572788 au

No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.892620	−0.761794	1.173072
2	6	0	7.425171	−2.059680	0.725577
3	6	0	7.425173	−2.059793	−0.725257
4	6	0	7.892623	−0.761976	−1.172951
5	6	0	8.175911	0.039483	−0.000001
6	6	0	5.785664	1.440158	−3.011480
7	6	0	7.026177	1.245524	−2.293947
8	6	0	7.320873	−0.175505	−2.292859
9	6	0	6.275592	−0.857793	−3.026970
10	6	0	5.317318	0.138905	−3.456364
11	6	0	5.817472	−2.095117	2.588348
12	6	0	4.411776	−2.417665	2.601874
13	6	0	4.129370	−3.198317	1.421221
14	6	0	5.368637	−3.400153	0.693596
15	6	0	6.418314	−2.712886	1.418005
16	6	0	3.015328	0.851075	−2.995200
17	6	0	3.959030	−0.144681	−3.441894
18	6	0	3.479943	−1.446685	−2.995876
19	6	0	2.232324	−1.270905	−2.320900
20	6	0	1.961682	0.172729	−2.277655
21	6	0	3.460765	2.104678	−2.583815
22	6	0	2.877917	2.714779	−1.422403
23	6	0	3.934083	3.400425	−0.691991
24	6	0	5.172390	3.202453	−1.415136
25	6	0	4.878125	2.400499	−2.587607
26	6	0	7.320865	−0.175150	2.292888
27	6	0	7.026168	1.245879	2.293753
28	6	0	5.785655	1.440624	3.011253
29	6	0	5.317307	0.139441	3.456337
30	6	0	6.275581	−0.857324	3.027098
31	6	0	6.418317	−2.713105	−1.417586
32	6	0	5.368640	−3.400263	−0.693076
33	6	0	4.129375	−3.198539	−1.420735
34	6	0	4.411785	−2.418069	−2.601509
35	6	0	5.817479	−2.095517	−2.588027
36	6	0	7.900992	1.400736	−0.000108
37	6	0	7.308330	2.012759	−1.171728
38	6	0	6.361654	3.014052	−0.724561
39	6	0	6.361651	3.014165	0.724092
40	6	0	7.308323	2.012937	1.171415
41	6	0	3.934081	3.400536	0.691456

42	6	0	2.877913	2.714998	1.421967
43	6	0	3.460757	2.105078	2.583477
44	6	0	4.878117	2.400902	2.587229
45	6	0	5.172385	3.202676	1.414634
46	6	0	1.989783	−1.988473	1.139274
47	6	0	1.353334	−1.436800	0.000100
48	6	0	1.989788	−1.988648	−1.138980
49	6	0	2.950188	−3.005572	−0.717014
50	6	0	2.950185	−3.005461	0.717467
51	6	0	3.015318	0.851539	2.995054
52	6	0	1.961676	0.173083	2.277609
53	6	0	2.232318	−1.270544	2.321078
54	6	0	3.479934	−1.446221	2.996088
55	6	0	3.959019	−0.144149	3.441904
56	6	0	1.385199	0.764910	−1.176200
57	6	0	0.788519	−0.026848	−0.000009
58	6	0	1.385198	0.765094	1.176059
59	6	0	1.887365	2.028650	0.725477
60	6	0	1.887367	2.028535	−0.725811
61	6	0	−1.989786	1.988480	−1.139269
62	6	0	−2.950188	3.005466	−0.717451
63	6	0	−2.950185	3.005567	0.717030
64	6	0	−1.989785	1.988641	1.138985
65	6	0	−1.353334	1.436800	−0.000107
66	6	0	−3.015314	−0.851098	2.995186
67	6	0	−1.961671	−0.172747	2.277642
68	6	0	−2.232317	1.270887	2.320895
69	6	0	−3.479931	1.446662	2.995883
70	6	0	−3.959014	0.144655	3.441892
71	6	0	−4.411788	2.417686	−2.601857
72	6	0	−5.817482	2.095136	−2.588325
73	6	0	−6.418319	2.712896	−1.417975
74	6	0	−5.368640	3.400158	−0.693565
75	6	0	−4.129376	3.198326	−1.421197
76	6	0	−5.785650	−1.440181	3.011474
77	6	0	−5.317302	−0.138932	3.456367
78	6	0	−6.275578	0.857769	3.026983
79	6	0	−7.320863	0.175487	2.292873
80	6	0	−7.026166	−1.245542	2.293949
81	6	0	−4.878113	−2.400520	2.587590
82	6	0	−5.172384	−3.202464	1.415114
83	6	0	−3.934080	−3.400431	0.691962
84	6	0	−2.877910	−2.714789	1.422373
85	6	0	−3.460753	−2.104697	2.583793
86	6	0	−2.232325	1.270563	−2.321084
87	6	0	−1.961686	−0.173065	−2.277623
88	6	0	−3.015332	−0.851517	−2.995068
89	6	0	−3.959035	0.144175	−3.441907
90	6	0	−3.479946	1.446244	−2.996081
91	6	0	−4.129369	3.198530	1.420759
92	6	0	−5.368637	3.400258	0.693107
93	6	0	−6.418312	2.713094	1.417616
94	6	0	−5.817469	2.095498	2.588050
95	6	0	−4.411773	2.418049	2.601526
96	6	0	−0.788519	0.026848	−0.000009
97	6	0	−1.385195	−0.764919	1.176178
98	6	0	−1.887363	−2.028541	0.725782
99	6	0	−1.887368	−2.028643	−0.725507
100	6	0	−1.385202	−0.765085	−1.176081
101	6	0	−3.934084	−3.400530	−0.691485
102	6	0	−5.172393	−3.202665	−1.414657
103	6	0	−4.878128	−2.400882	−2.587246
104	6	0	−3.460768	−2.105059	−2.583499
105	6	0	−2.877919	−2.714988	−1.421997
106	6	0	−7.892626	0.761803	−1.173051
107	6	0	−8.175911	−0.039484	0.000017
108	6	0	−7.892617	0.761967	1.172971
109	6	0	−7.425170	2.059788	0.725286
110	6	0	−7.425174	2.059685	−0.725548
111	6	0	−5.785668	−1.440601	−3.011258
112	6	0	−7.026178	−1.245861	−2.293751
113	6	0	−7.320875	0.175168	−2.292874
114	6	0	−6.275596	0.857347	−3.027085
115	6	0	−5.317322	−0.139414	−3.456335
116	6	0	−7.308325	−2.012768	1.171725
117	6	0	−7.900993	−1.400737	0.000112
118	6	0	−7.308329	−2.012928	−1.171418
119	6	0	−6.361654	−3.014159	−0.724107
120	6	0	−6.361651	−3.014058	0.724546

C_{60}^- dimer (triplet) by UωB97XD/6-31G(d)/SMD(oDCB)

E(UwB97XD) = −4571.25372364 au (*C*1 symmetry)
Sum of electronic and thermal Free Energies= −4570.569987 au
No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−8.333186	0.065173	0.360351
2	6	0	−8.335182	−0.555901	−0.933196
3	6	0	−8.196788	−1.986848	−0.742495
4	6	0	−8.128503	−2.252941	0.681288
5	6	0	−8.197987	−0.977923	1.362698
6	6	0	−5.226813	−3.674241	2.171805
7	6	0	−6.509973	−3.028674	2.357013
8	6	0	−7.299394	−3.257924	1.164650
9	6	0	−6.505277	−4.044848	0.246616
10	6	0	−5.225944	−4.302633	0.868344
11	6	0	−7.008134	1.325628	−1.807902
12	6	0	−5.802961	1.335669	−2.614414
13	6	0	−5.726272	0.059726	−3.292041
14	6	0	−6.895134	−0.721897	−2.921847
15	6	0	−7.685449	0.059525	−2.013775
16	6	0	−2.865366	−3.665172	0.598816
17	6	0	−4.066718	−4.297791	0.098069
18	6	0	−4.139099	−4.030250	−1.324029
19	6	0	−2.970891	−3.255529	−1.703135
20	6	0	−2.190855	−3.025662	−0.517958
21	6	0	−2.866228	−3.062718	1.848471
22	6	0	−2.191824	−1.795464	2.052730
23	6	0	−2.981549	−1.012940	2.963724
24	6	0	−4.149023	−1.794503	3.333115
25	6	0	−4.071879	−3.071211	2.654455
26	6	0	−7.685750	1.289902	0.558654
27	6	0	−6.905780	1.518790	1.741680
28	6	0	−5.736936	2.294682	1.362994
29	6	0	−5.808698	2.562525	−0.058130
30	6	0	−7.008959	1.928343	−0.558358
31	6	0	−7.435078	−2.742017	−1.622128
32	6	0	−6.766501	−2.103707	−2.744480
33	6	0	−5.495573	−2.745735	−2.929107
34	6	0	−5.366909	−3.782168	−1.920507
35	6	0	−6.575105	−3.791652	−1.120216
36	6	0	−7.444160	−0.757781	2.505236
37	6	0	−6.581494	−1.806320	3.011133
38	6	0	−5.376832	−1.175026	3.511212
39	6	0	−5.507731	0.258946	3.329049
40	6	0	−6.778343	0.515128	2.710559
41	6	0	−3.110574	0.367063	2.783985
42	6	0	−2.440815	1.006472	1.663500
43	6	0	−3.300739	2.055733	1.160701
44	6	0	−4.509627	2.046165	1.960337
45	6	0	−4.381561	1.010585	2.969633
46	6	0	−3.293122	0.070131	−2.970922
47	6	0	−2.430225	−0.978577	−2.466287
48	6	0	−3.098712	−2.251135	−2.669421
49	6	0	−4.368649	−1.994820	−3.289840
50	6	0	−4.498812	−0.560865	−3.469834
51	6	0	−3.369808	2.308803	−0.205515
52	6	0	−2.574927	1.521000	−1.124001
53	6	0	−3.364556	1.292412	−2.316784
54	6	0	−4.646850	1.938779	−2.131018
55	6	0	−4.647973	2.567001	−0.828580
56	6	0	−1.545856	−1.802624	−0.320909
57	6	0	−1.679276	−0.760012	−1.322351
58	6	0	−1.751379	0.514515	−0.640138
59	6	0	−1.684017	0.249439	0.783323
60	6	0	−1.547357	−1.180456	0.973956
61	6	0	3.135110	2.254842	−2.713845
62	6	0	4.412976	1.997957	−3.317194
63	6	0	4.544310	0.563691	−3.496737
64	6	0	3.331898	−0.066745	−3.014633
65	6	0	2.463677	0.982316	−2.520002
66	6	0	3.370282	−2.307800	−0.250269
67	6	0	2.588229	−1.518948	−1.178688
68	6	0	3.393686	−1.290047	−2.360588
69	6	0	4.672792	−1.937322	−2.159078
70	6	0	4.656716	−2.566369	−0.856960
71	6	0	5.394450	3.784016	−1.934633
72	6	0	6.592051	3.791862	−1.118809
73	6	0	7.457727	2.741492	−1.610682
74	6	0	6.803828	2.105124	−2.742329
75	6	0	5.535652	2.747807	−2.942197

76	6	0	5.717046	−2.297192	1.348869
77	6	0	5.806813	−2.563368	−0.071690
78	6	0	7.014428	−1.929624	−0.555710
79	6	0	7.677373	−1.293370	0.570368
80	6	0	6.881400	−1.522075	1.742493
81	6	0	4.482319	−2.048268	1.930253
82	6	0	4.341748	−1.012940	2.938544
83	6	0	3.073628	−0.368650	2.737413
84	6	0	2.418577	−1.006101	1.607521
85	6	0	3.283984	−2.056146	1.115006
86	6	0	2.995521	3.258596	−1.748308
87	6	0	2.199494	3.028751	−0.574055
88	6	0	2.860053	3.666223	0.551843
89	6	0	4.068705	4.298380	0.067341
90	6	0	4.159175	4.032504	−1.354158
91	6	0	5.769010	−0.057616	−3.303754
92	6	0	6.933569	0.722752	−2.919113
93	6	0	7.710398	−0.059663	−2.000615
94	6	0	7.029974	−1.326270	−1.804648
95	6	0	5.835684	−1.334615	−2.626434
96	6	0	1.697067	0.763515	−1.386567
97	6	0	1.758985	−0.511947	−0.704674
98	6	0	1.674342	−0.248054	0.717566
99	6	0	1.536721	1.182201	0.907537
100	6	0	1.551243	1.805505	−0.386468
101	6	0	2.943444	1.011804	2.916546
102	6	0	4.106554	1.792122	3.300559
103	6	0	4.039410	3.069857	2.622185
104	6	0	2.844596	3.063002	1.800845
105	6	0	2.167078	1.795352	1.995178
106	6	0	8.120956	2.250132	0.701312
107	6	0	8.180472	0.974217	1.382354
108	6	0	8.328054	−0.068418	0.381357
109	6	0	8.346270	0.553823	−0.911302
110	6	0	8.207011	1.985345	−0.721335
111	6	0	5.201068	3.672474	2.155472
112	6	0	6.481157	3.026014	2.356408
113	6	0	7.286285	3.255611	1.174999
114	6	0	6.504898	4.043559	0.247038
115	6	0	5.217372	4.301825	0.852435
116	6	0	6.742251	−0.519099	2.710636
117	6	0	7.410963	0.753814	2.514409
118	6	0	6.543059	1.802628	3.010429
119	6	0	5.331650	1.171893	3.493824
120	6	0	5.463725	−0.262322	3.312133

TD-DFT

Ground state optimization for Li⁺@C_{60}^- dimer (singlet)
by wB97XD/6-31G(d)/IEFPCM(oDCB)
E(RwB97XD) = −4586.12432752 au (*C*1 symmetry)
Sum of electronic and thermal Free Energies= −4585.412815 au
No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.868690	−0.797040	1.223506
2	6	0	7.412837	−2.079189	0.723212
3	6	0	7.446784	−2.031311	−0.726713
4	6	0	7.923490	−0.719431	−1.120910
5	6	0	8.180219	0.043577	0.084266
6	6	0	5.858119	1.541532	−2.932779
7	6	0	7.085526	1.325997	−2.197107
8	6	0	7.378480	−0.095848	−2.233209
9	6	0	6.347642	−0.754953	−3.009194
10	6	0	5.398108	0.255127	−3.426278
11	6	0	5.765144	−2.176996	2.547764
12	6	0	4.354913	−2.498089	2.515700
13	6	0	4.100471	−3.239187	1.306337
14	6	0	5.356083	−3.413099	0.599267
15	6	0	6.390376	−2.753901	1.370941
16	6	0	3.087786	0.952611	−3.004356
17	6	0	4.041326	−0.029372	−3.466894
18	6	0	3.554034	−1.346919	−3.076244
19	6	0	2.290749	−1.191125	−2.419465
20	6	0	2.013854	0.251905	−2.332875
21	6	0	3.524546	2.186566	−2.534596
22	6	0	2.915177	2.756050	−1.365456
23	6	0	3.952605	3.423252	−0.593430
24	6	0	5.206839	3.253110	−1.296268
25	6	0	4.941356	2.487858	−2.499508
26	6	0	7.273179	−0.246998	2.349011
27	6	0	6.975549	1.173647	2.390271
28	6	0	5.718538	1.345586	3.086220
29	6	0	5.240245	0.030313	3.474658
30	6	0	6.208406	−0.952788	3.031233
31	6	0	6.456489	−2.661401	−1.462558
32	6	0	5.389605	−3.369651	−0.785195
33	6	0	4.166863	−3.152155	−1.539756
34	6	0	4.476022	−2.328236	−2.683007
35	6	0	5.884236	−2.007523	−2.626698
36	6	0	7.899148	1.402165	0.122332
37	6	0	7.340393	2.057594	−1.043960
38	6	0	6.379553	3.041791	−0.584497
39	6	0	6.344332	2.994865	0.864166
40	6	0	7.277236	1.975109	1.298712
41	6	0	3.919665	3.379340	0.787959
42	6	0	2.848830	2.666959	1.466936
43	6	0	3.404286	2.021894	2.624394
44	6	0	4.820991	2.320353	2.673196
45	6	0	5.140688	3.162979	1.535899
46	6	0	1.963642	−2.028385	1.020579
47	6	0	1.362370	−1.425008	−0.122491
48	6	0	2.012531	−1.955359	−1.273247
49	6	0	2.966249	−2.983651	−0.855883
50	6	0	2.932837	−3.028486	0.581093
51	6	0	2.949624	0.757578	2.986488
52	6	0	1.909375	0.104161	2.224436
53	6	0	2.184037	−1.342429	2.223912
54	6	0	3.417173	−1.540016	2.921167
55	6	0	3.884484	−0.253175	3.419495
56	6	0	1.404704	0.810352	−1.226437
57	6	0	0.783511	−0.020696	−0.085947
58	6	0	1.356242	0.734229	1.130477
59	6	0	1.865796	2.016018	0.731207
60	6	0	1.897869	2.061681	−0.719430
61	3	0	3.552717	−0.397176	−0.162497
62	6	0	−2.012446	1.955080	−1.273476
63	6	0	−2.966111	2.983477	−0.856233
64	6	0	−2.932677	3.028491	0.580741
65	6	0	−1.963522	2.028391	1.020332
66	6	0	−1.362297	1.424839	−0.122664
67	6	0	−2.949622	−0.757305	2.986622
68	6	0	−1.909358	−0.104034	2.224463
69	6	0	−2.183952	1.342567	2.223732
70	6	0	−3.417066	1.540294	2.920965
71	6	0	−3.884431	0.253553	3.419498
72	6	0	−4.475951	2.327880	−2.683235
73	6	0	−5.884177	2.007243	−2.626874
74	6	0	−6.456388	2.661302	−1.462814
75	6	0	−5.389461	3.369596	−0.785554
76	6	0	−4.166734	3.151955	−1.540110
77	6	0	−5.718563	−1.345153	3.086460
78	6	0	−5.240205	−0.029854	3.474737
79	6	0	−6.208319	0.953239	3.031186
80	6	0	−7.273139	0.247419	2.349074
81	6	0	−6.975571	−1.173234	2.390505
82	6	0	−4.821070	−2.320023	2.673556
83	6	0	−5.140826	−3.162777	1.536369
84	6	0	−3.919823	−3.379282	0.788437
85	6	0	−2.848938	−2.666885	1.467313
86	6	0	−3.404350	−2.021644	2.624697
87	6	0	−2.290729	1.190699	−2.419582
88	6	0	−2.013899	−0.252332	−2.332811
89	6	0	−3.087871	−0.953072	−3.004191
90	6	0	−4.041369	0.028895	−3.466846
91	6	0	−3.554017	1.346466	−3.076354
92	6	0	−4.100295	3.239338	1.305977
93	6	0	−5.355911	3.413211	0.598900
94	6	0	−6.390224	2.754153	1.370671
95	6	0	−5.765002	2.177363	2.547551
96	6	0	−4.354755	2.498372	2.515410
97	6	0	−0.783515	0.020498	−0.085941
98	6	0	−1.356267	−0.734262	1.130579
99	6	0	−1.865883	−2.016082	0.731487
100	6	0	−1.897990	−2.061907	−0.719142
101	6	0	−1.404759	−0.810669	−1.226314
102	6	0	−3.952783	−3.423368	−0.592944
103	6	0	−5.207017	−3.253254	−1.295785
104	6	0	−4.941511	−2.488167	−2.499125
105	6	0	−3.524686	−2.186949	−2.534275
106	6	0	−2.915332	−2.756316	−1.365072

107	6	0	−7.923474	0.719444	−1.120901
108	6	0	−8.180218	−0.043400	0.084375
109	6	0	−7.868632	0.797346	1.223504
110	6	0	−7.412725	2.079409	0.723041
111	6	0	−7.446705	2.031354	−0.726878
112	6	0	−5.858233	−1.541852	−2.932498
113	6	0	−7.085622	−1.326164	−2.196842
114	6	0	−7.378509	0.095691	−2.233127
115	6	0	−6.347649	0.754645	−3.009210
116	6	0	−5.398166	−0.255535	−3.426174
117	6	0	−7.277309	−1.974818	1.299054
118	6	0	−7.899217	−1.401998	0.122613
119	6	0	−7.340512	−2.057606	−1.043602
120	6	0	−6.379712	−3.041788	−0.584027
121	6	0	−6.344470	−2.994685	0.864631
122	3	0	−3.552724	0.397117	−0.162253

TD excitation wavelength (nstates=20)

Excited State	1: 811.38 nm	f=0.0155
Excited State	2: 796.60 nm	f=0.0011
Excited State	3: 772.21 nm	f=0.0278
Excited State	4: 763.98 nm	f=0.0001
Excited State	5: 571.61 nm	f=0.1719
Excited State	6: 546.43 nm	f=0.0000
Excited State	7: 470.10 nm	f=0.0000
Excited State	8: 470.10 nm	f=0.0000
Excited State	9: 467.99 nm	f=0.0002
Excited State	10: 467.82 nm	f=0.0059
Excited State	11: 462.88 nm	f=0.0005
Excited State	12: 461.79 nm	f=0.0065
Excited State	13: 451.58 nm	f=0.0001
Excited State	14: 450.73 nm	f=0.0061
Excited State	15: 448.50 nm	f=0.0026
Excited State	16: 445.75 nm	f=0.0013
Excited State	17: 442.38 nm	f=0.0000
Excited State	18: 441.69 nm	f=0.0003
Excited State	19: 438.96 nm	f=0.0000
Excited State	20: 436.20 nm	f=0.0432

Ground state optimization for $Li^{+}@C_{60}^{-}$ monomer (doublet)
by UwB97XD/6-31G(d)/IEFPCM(oDCB)

E(UwB97XD) = −2293.03803339 au (*C*1 symmetry)
Sum of electronic and thermal Free Energies= −2292.699217au
No imaginary frequency on IR calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.021904	0.421080	3.362895
2	6	0	2.265300	0.037629	2.716070
3	6	0	2.734258	1.167567	1.938870
4	6	0	1.762361	2.235801	2.092898
5	6	0	0.717416	1.779475	2.985685
6	6	0	−0.134744	3.472691	−0.654850
7	6	0	0.078499	3.449299	0.770704
8	6	0	1.456686	3.055720	1.016055
9	6	0	2.096172	2.835955	−0.261846
10	6	0	1.108355	3.083797	−1.293375
11	6	0	1.374449	−2.230307	2.385468
12	6	0	1.353585	−3.039723	1.200880
13	6	0	2.408008	−2.580865	0.316677
14	6	0	3.085454	−1.472207	0.963394
15	6	0	2.439982	−1.254533	2.245337
16	6	0	−0.180132	1.866068	−3.001354
17	6	0	1.085480	2.298254	−2.435636
18	6	0	2.041686	1.221074	−2.582861
19	6	0	1.370001	0.124783	−3.230458
20	6	0	−0.008436	0.527581	−3.491826
21	6	0	−1.380829	2.238052	−2.380282
22	6	0	−2.443818	1.265735	−2.237406
23	6	0	−3.084897	1.482793	−0.950509
24	6	0	−2.403035	2.586750	−0.302735
25	6	0	−1.350015	3.045136	−1.190219
26	6	0	0.002563	−0.518041	3.497825
27	6	0	−1.374736	−0.120724	3.251551
28	6	0	−2.046992	−1.220188	2.599345
29	6	0	−1.087212	−2.295564	2.445898
30	6	0	0.177136	−1.864551	3.011796
31	6	0	3.347843	0.959622	0.711784
32	6	0	3.527247	−0.391653	0.214107
33	6	0	3.317614	−0.368089	−1.220387
34	6	0	3.003556	0.990160	−1.601813
35	6	0	3.032270	1.815657	−0.415568
36	6	0	−0.607007	2.158264	2.748156
37	6	0	−0.926662	3.003085	1.622894
38	6	0	−2.191810	2.561149	1.066823
39	6	0	−2.652864	1.434781	1.850704
40	6	0	−1.669258	1.186247	2.889992
41	6	0	−3.523355	0.403023	−0.199880
42	6	0	−3.357513	−0.950311	−0.695838
43	6	0	−3.043794	−1.806006	0.426183
44	6	0	−2.998573	−0.983573	1.613750
45	6	0	−3.308383	0.381058	1.235058
46	6	0	0.933089	−2.998900	−1.619738
47	6	0	0.614558	−2.164449	−2.742895
48	6	0	1.671554	−1.181844	−2.869594
49	6	0	2.669494	−1.433102	−1.841522
50	6	0	2.206822	−2.558113	−1.058349
51	6	0	−2.103126	−2.832116	0.271386
52	6	0	−1.461645	−3.042002	−1.002625
53	6	0	−0.078725	−3.443495	−0.758412
54	6	0	0.132212	−3.456653	0.658563
55	6	0	−1.113489	−3.078802	1.300498
56	6	0	−1.029890	−0.417792	−3.352118
57	6	0	−0.726355	−1.773757	−2.983726
58	6	0	−1.770600	−2.224744	−2.086379
59	6	0	−2.748578	−1.157777	−1.933168
60	6	0	−2.283631	−0.031607	−2.714244
61	3	0	−0.005220	−0.675175	−0.673200

TD excitation wavelength (nstates=20)

Excited State	1: 4847.56 nm	f=0.0000
Excited State	2: 4143.01 nm	f=0.0005
Excited State	3: 1028.57 nm	f=0.0619
Excited State	4: 1004.38 nm	f=0.0588
Excited State	5: 731.04 nm	f=0.0000
Excited State	6: 658.27 nm	f=0.0003
Excited State	7: 654.46 nm	f=0.0000
Excited State	8: 643.90 nm	f=0.0002
Excited State	9: 515.82 nm	f=0.0006
Excited State	10: 512.05 nm	f=0.0004
Excited State	11: 510.44 nm	f=0.0006
Excited State	12: 497.87 nm	f=0.0010
Excited State	13: 496.47 nm	f=0.0005
Excited State	14: 486.49 nm	f=0.0059
Excited State	15: 484.57 nm	f=0.0006
Excited State	16: 482.35 nm	f=0.0002
Excited State	17: 475.93 nm	f=0.0004
Excited State	18: 473.67 nm	f=0.0016
Excited State	19: 472.23 nm	f=0.0023
Excited State	20: 469.00 nm	f=0.0003