

Electronic Supplementary Information

Encapsulation of diatomic molecules in fullerene C₆₀: Implications for their main properties

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Cartesian coordinates (in Å) of DF-LMP2/cc-pVTZ optimized structures of endohedral fullerene complexes of C₆₀ with the following guest molecules: H₂, N₂, O₂, F₂, HF, CO, LiH, LiF, BN and BeO.

 Format:

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{Total_number_of_atoms}
{Comment_line}
{Atom_line_number} {Atom} {X} {Y} {Z}
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 DF-LMP2/VTZ optimized structure of H2@C60 (D5d)

1	C	0.8901374382	0.0649346510	-0.8465710110
2	C	-0.3400022467	0.8252027872	-0.8465710110
3	C	-1.1002703829	0.4450687191	0.3233613523
4	C	-0.3400022467	-0.5501351915	1.0464193174
5	C	0.8901374382	-0.7850709658	0.3233613523
6	C	0.8901374382	0.0649346510	4.3435257922
7	C	0.8901374382	-0.7850709658	3.1735934289
8	C	-0.3400022467	-0.5501351915	2.4505354639
9	C	-1.1002703829	0.4450687191	3.1735934289
10	C	-0.3400022467	0.8252027872	4.3435257922
11	C	0.8901374382	2.7756664404	-1.7273411606
12	C	0.8901374382	4.1510044191	-1.2804667623
13	C	-0.3400022467	4.3859401935	-0.5574087973
14	C	-1.1002703829	3.1558005085	-0.5574087973
15	C	-0.3400022467	2.1605965980	-1.2804667623
16	C	0.8901374382	2.7756664404	5.2242959418
17	C	-0.3400022467	2.1605965980	4.7774215436
18	C	-1.1002703829	3.1558005085	4.0543635785
19	C	-0.3400022467	4.3859401935	4.0543635785
20	C	0.8901374382	4.1510044191	4.7774215436
21	C	2.0845499732	2.0374788972	5.2242959418
22	C	3.3146896582	2.6525487397	4.7774215436
23	C	4.0749577944	1.6573448291	4.0543635785
24	C	3.3146896582	0.4272051442	4.0543635785
25	C	2.0845499732	0.6621409185	4.7774215436
26	C	2.0845499732	0.6621409185	-1.2804667623
27	C	3.3146896582	0.4272051442	-0.5574087973
28	C	4.0749577944	1.6573448291	-0.5574087973
29	C	3.3146896582	2.6525487397	-1.2804667623
30	C	2.0845499732	2.0374788972	-1.7273411606
31	C	-1.8384579262	1.4113687582	1.0254194256
32	C	-1.8384579262	2.7867067369	0.5785450273
33	C	-1.8384579262	3.6367123537	1.7484773906
34	C	-1.8384579262	2.7867067369	2.9184097539
35	C	-1.8384579262	1.4113687582	2.4715353557
36	C	2.0845499732	-1.0131834617	1.0254194256
37	C	2.0845499732	-1.0131834617	2.4715353557
38	C	3.3146896582	-0.3981136193	2.9184097539
39	C	4.0749577944	-0.0179795512	1.7484773906
40	C	3.3146896582	-0.3981136193	0.5785450273
41	C	4.8131453376	2.0264386007	2.9184097539
42	C	4.8131453376	3.4017765794	2.4715353557
43	C	4.8131453376	3.4017765794	1.0254194256
44	C	4.8131453376	2.0264386007	0.5785450273
45	C	4.8131453376	1.1764329839	1.7484773906
46	C	0.8901374382	5.8263287993	1.0254194256
47	C	0.8901374382	5.8263287993	2.4715353557

48	C	-0.3400022467	5.2112589569	2.9184097539
49	C	-1.1002703829	4.8311248888	1.7484773906
50	C	-0.3400022467	5.2112589569	0.5785450273
51	C	4.0749577944	4.3680766185	0.3233613523
52	C	3.3146896582	5.3632805291	1.0464193174
53	C	2.0845499732	5.5982163034	0.3233613523
54	C	2.0845499732	4.7482106866	-0.8465710110
55	C	3.3146896582	3.9879425504	-0.8465710110
56	C	2.0845499732	4.7482106866	4.3435257922
57	C	2.0845499732	5.5982163034	3.1735934289
58	C	3.3146896582	5.3632805291	2.4505354639
59	C	4.0749577944	4.3680766185	3.1735934289
60	C	3.3146896582	3.9879425504	4.3435257922
61	H	1.3207363327	2.1369962765	1.5526186771
62	H	1.6539510787	2.6761490611	1.9443361042

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DF-LMP2/VTZ optimized structure of N2@C60 (D5d)

1	C	0.8901770097	0.0649375377	-0.8466086457
2	C	-0.3400173617	0.8252394720	-0.8466086457
3	C	-1.1003192960	0.4450885048	0.3233757275
4	C	-0.3400173617	-0.5501596480	1.0464658364
5	C	0.8901770097	-0.7851058665	0.3233757275
6	C	0.8901770097	0.0649375377	4.3441040668
7	C	0.8901770097	-0.7851058665	3.1741196936
8	C	-0.3400173617	-0.5501596480	2.4510295847
9	C	-1.1003192960	0.4450885048	3.1741196936
10	C	-0.3400173617	0.8252394720	4.3441040668
11	C	0.8901770097	2.7761561630	-1.7275369779
12	C	0.8901770097	4.1515552830	-1.2806427136
13	C	-0.3400173617	4.3865015015	-0.5575526047
14	C	-1.1003192960	3.1563071301	-0.5575526047
15	C	-0.3400173617	2.1610589773	-1.2806427136
16	C	0.8901770097	2.7761561630	5.2250323990
17	C	-0.3400173617	2.1610589773	4.7781381347
18	C	-1.1003192960	3.1563071301	4.0550480258
19	C	-0.3400173617	4.3865015015	4.0550480258
20	C	0.8901770097	4.1515552830	4.7781381347
21	C	2.0849702975	2.0377333016	5.2250323990
22	C	3.3151646689	2.6528304873	4.7781381347
23	C	4.0754666032	1.6575823344	4.0550480258
24	C	3.3151646689	0.4273879631	4.0550480258
25	C	2.0849702975	0.6623341816	4.7781381347
26	C	2.0849702975	0.6623341816	-1.2806427136
27	C	3.3151646689	0.4273879631	-0.5575526047
28	C	4.0754666032	1.6575823344	-0.5575526047
29	C	3.3151646689	2.6528304873	-1.2806427136
30	C	2.0849702975	2.0377333016	-1.7275369779
31	C	-1.8387421574	1.4116965795	1.0256576016
32	C	-1.8387421574	2.7870956994	0.5787633374
33	C	-1.8387421574	3.6371391037	1.7487477106
34	C	-1.8387421574	2.7870956994	2.9187320838
35	C	-1.8387421574	1.4116965795	2.4718378195
36	C	2.0849702975	-1.0132910797	1.0256576016
37	C	2.0849702975	-1.0132910797	2.4718378195
38	C	3.3151646689	-0.3981938941	2.9187320838
39	C	4.0754666032	-0.0180429269	1.7487477106
40	C	3.3151646689	-0.3981938941	0.5787633374

41	C	4.8138894646	2.0267937651	2.9187320838
42	C	4.8138894646	3.4021928851	2.4718378195
43	C	4.8138894646	3.4021928851	1.0256576016
44	C	4.8138894646	2.0267937651	0.5787633374
45	C	4.8138894646	1.1767503609	1.7487477106
46	C	0.8901770097	5.8271805443	1.0256576016
47	C	0.8901770097	5.8271805443	2.4718378195
48	C	-0.3400173617	5.2120833586	2.9187320838
49	C	-1.1003192960	4.8319323915	1.7487477106
50	C	-0.3400173617	5.2120833586	0.5787633374
51	C	4.0754666032	4.3688009597	0.3233757275
52	C	3.3151646689	5.3640491126	1.0464658364
53	C	2.0849702975	5.5989953311	0.3233757275
54	C	2.0849702975	4.7489519269	-0.8466086457
55	C	3.3151646689	3.9886499926	-0.8466086457
56	C	2.0849702975	4.7489519269	4.3441040668
57	C	2.0849702975	5.5989953311	3.1741196936
58	C	3.3151646689	5.3640491126	2.4510295847
59	C	4.0754666032	4.3688009597	3.1741196936
60	C	3.3151646689	3.9886499926	4.3441040668
61	N	1.2369225509	2.0013827288	1.4540896673
62	N	1.7382247563	2.8125067358	2.0434057538

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DF-LMP2/VTZ optimized structure of O2@C60 (Ci)

1	C	-0.5977466690	-2.3449641598	-2.5991102037
2	C	-1.8284038586	-1.5851464289	-2.5985276760
3	C	-2.5909648463	-1.9660899517	-1.4290841736
4	C	-1.8300937017	-2.9608781859	-0.7059074168
5	C	-0.5985104819	-3.1945759035	-1.4289349618
6	C	-0.5993580741	-2.3404664609	2.5917071677
7	C	-0.5993185893	-3.1905807588	1.4219783337
8	C	-1.8306175821	-2.9586192281	0.6993343572
9	C	-2.5922906160	-1.9648331100	1.4238383099
10	C	-1.8303049105	-1.5823794407	2.5923365488
11	C	-0.5959459973	0.3678118701	-3.4751724830
12	C	-0.5948950360	1.7423784014	-3.0264143045
13	C	-1.8251321548	1.9764015188	-2.3038697780
14	C	-2.5858247703	0.7464010325	-2.3054758712
15	C	-1.8262186103	-0.2483692995	-3.0299889053
16	C	-0.5985938430	0.3692979205	3.4743638592
17	C	-1.8280680603	-0.2469471263	3.0265402927
18	C	-2.5878835559	0.7475206391	2.3037617001
19	C	-1.8272883146	1.9776668812	2.3056134191
20	C	-0.5974677303	1.7450024816	3.0295384048
21	C	0.5959730382	-0.3677817710	3.4752130620
22	C	1.8262485348	0.2483983232	3.0300321393
23	C	2.5858511246	-0.7463708137	2.3055126349
24	C	1.8251565128	-1.9763694973	2.3039042127
25	C	0.5949196466	-1.7423475459	3.0264513934
26	C	0.5974933888	-1.7449772499	-3.0295046357
27	C	1.8273146082	-1.9776381533	-2.3055781993
28	C	2.5879099262	-0.7474914286	-2.3037246682
29	C	1.8280939385	0.2469744940	-3.0265037221
30	C	0.5986189062	-0.3692701977	-3.4743259777
31	C	-3.3291543867	-0.9994927260	-0.7247889916
32	C	-3.3253825699	0.3766986793	-1.1701435650
33	C	-3.3248456234	1.2266978786	-0.0002532501

34	C	-3.3272904666	0.3766314236	1.1688776816
35	C	-3.3310284386	-0.9990274800	0.7218597278
36	C	0.5965421133	-3.4196970883	-0.7257711624
37	C	0.5957915476	-3.4181202707	0.7203056739
38	C	1.8252046191	-2.8018272455	1.1678616262
39	C	2.5861117267	-2.4213513813	-0.0010482716
40	C	1.8268337946	-2.8035488953	-1.1707805931
41	C	3.3254136505	-0.3766705556	1.1701801063
42	C	3.3291909514	0.9995213133	0.7248249883
43	C	3.3310610181	0.9990555814	-0.7218232904
44	C	3.3273228080	-0.3766028546	-1.1688432496
45	C	3.3248745942	-1.2266695492	0.0002879919
46	C	-0.5957682718	3.4181486741	-0.7202713678
47	C	-0.5965165408	3.4197182245	0.7258032071
48	C	-1.8268092507	2.8035764273	1.1708148680
49	C	-2.5860890339	2.4213827066	0.0010820580
50	C	-1.8251820547	2.8018607061	-1.1678285340
51	C	2.5923150604	1.9648562444	-1.4238018749
52	C	1.8306378598	2.9586374153	-0.6992976193
53	C	0.5993423098	3.1906062004	-1.4219411356
54	C	0.5993826313	2.3404960595	-2.5916716520
55	C	1.8303297572	1.5824060571	-2.5923003711
56	C	0.5977731112	2.3449821302	2.5991404999
57	C	0.5985345453	3.1945875289	1.4289636671
58	C	1.8301160145	2.9608908002	0.7059414053
59	C	2.5909949911	1.9661129152	1.4291216521
60	C	1.8284350738	1.5851727727	2.5985663415
61	O	-0.4282901147	-0.4267812141	-0.1915492916
62	O	0.4287091032	0.4259776709	0.1916716190

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DF-LMP2/VTZ optimized structure of F2@C60 (D2h)

1	C	-1.170142361	3.029627393	-1.425458175
2	C	0.000000000	3.476582003	-0.702270382
3	C	1.170142361	3.029627393	-1.425458175
4	C	0.723187751	2.306439642	-2.595600605
5	C	-0.723187751	2.306439642	-2.595600605
6	C	1.425458091	-1.170142361	-3.029627570
7	C	0.702270340	0.000000000	-3.476582207
8	C	1.425458091	1.170142361	-3.029627570
9	C	2.595600453	0.723187751	-2.306439777
10	C	2.595600453	-0.723187751	-2.306439777
11	C	-1.170142361	3.029627393	1.425458175
12	C	-0.723187751	2.306439642	2.595600605
13	C	0.723187751	2.306439642	2.595600605
14	C	1.170142361	3.029627393	1.425458175
15	C	0.000000000	3.476582003	0.702270382
16	C	2.306439642	-2.595600453	-0.723187793
17	C	3.029627393	-1.425458091	-1.170142430
18	C	3.476582003	-0.702270340	0.000000000
19	C	3.029627393	-1.425458091	1.170142430
20	C	2.306439642	-2.595600453	0.723187793
21	C	1.170142361	-3.029627393	-1.425458175
22	C	0.000000000	-3.476582003	-0.702270382
23	C	-1.170142361	-3.029627393	-1.425458175
24	C	-0.723187751	-2.306439642	-2.595600605
25	C	0.723187751	-2.306439642	-2.595600605
26	C	-2.306439642	2.595600453	-0.723187793

27	C	-3.029627393	1.425458091	-1.170142430
28	C	-3.476582003	0.702270340	0.000000000
29	C	-3.029627393	1.425458091	1.170142430
30	C	-2.306439642	2.595600453	0.723187793
31	C	2.306439642	2.595600453	-0.723187793
32	C	2.306439642	2.595600453	0.723187793
33	C	3.029627393	1.425458091	1.170142430
34	C	3.476582003	0.702270340	0.000000000
35	C	3.029627393	1.425458091	-1.170142430
36	C	-1.425458091	1.170142361	-3.029627570
37	C	-0.702270340	0.000000000	-3.476582207
38	C	-1.425458091	-1.170142361	-3.029627570
39	C	-2.595600453	-0.723187751	-2.306439777
40	C	-2.595600453	0.723187751	-2.306439777
41	C	-2.306439642	-2.595600453	-0.723187793
42	C	-2.306439642	-2.595600453	0.723187793
43	C	-3.029627393	-1.425458091	1.170142430
44	C	-3.476582003	-0.702270340	0.000000000
45	C	-3.029627393	-1.425458091	-1.170142430
46	C	0.702270340	0.000000000	3.476582207
47	C	1.425458091	-1.170142361	3.029627570
48	C	2.595600453	-0.723187751	2.306439777
49	C	2.595600453	0.723187751	2.306439777
50	C	1.425458091	1.170142361	3.029627570
51	C	-2.595600453	-0.723187751	2.306439777
52	C	-1.425458091	-1.170142361	3.029627570
53	C	-0.702270340	0.000000000	3.476582207
54	C	-1.425458091	1.170142361	3.029627570
55	C	-2.595600453	0.723187751	2.306439777
56	C	1.170142361	-3.029627393	1.425458175
57	C	0.723187751	-2.306439642	2.595600605
58	C	-0.723187751	-2.306439642	2.595600605
59	C	-1.170142361	-3.029627393	1.425458175
60	C	0.000000000	-3.476582003	0.702270382
61	F	0.000000000	0.000000000	0.707193062
62	F	0.000000000	0.000000000	-0.707193063

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DF-LMP2/VTZ optimized structure of HF@C60 (C1)

1	C	-0.8942732251	0.0621068330	-0.8525650704
2	C	0.3354461092	0.8237089328	-0.8528067098
3	C	1.0950120717	0.4448833802	0.3188995329
4	C	0.3345229233	-0.5518405124	1.0425465930
5	C	-0.8950817211	-0.7879144603	0.3178633607
6	C	-0.8927675772	0.0618961505	4.3431836081
7	C	-0.8942538382	-0.7877098325	3.1727784763
8	C	0.3352449949	-0.5517732428	2.4482612878
9	C	1.0965620306	0.4441036342	3.1719470128
10	C	0.3370563210	0.8229553075	4.3432191431
11	C	-0.8936462006	2.7758530041	-1.7306292059
12	C	-0.8927334593	4.1508567529	-1.2837459475
13	C	0.3370786453	4.3857535452	-0.5607475040
14	C	1.0971772889	3.1558018250	-0.5609943263
15	C	0.3362154380	2.1603974388	-1.2843330279
16	C	-0.8918991583	2.7746421571	5.2217437949
17	C	0.3377254870	2.1593201797	4.7748838990
18	C	1.0982751571	3.1549057479	4.0517810157
19	C	0.3381444162	4.3847798392	4.0519287297

20	C	-0.8913570767	4.1497025526	4.7752704788
21	C	-2.0859539958	2.0363427509	5.2211293934
22	C	-3.3157732280	2.6513042641	4.7746088409
23	C	-4.0761446803	1.6566727916	4.0518272344
24	C	-3.3165531172	0.4266217219	4.0513739475
25	C	-2.0866819224	0.6610951247	4.7746318816
26	C	-2.0883863711	0.6617820256	-1.2833769294
27	C	-3.3179079295	0.4271500494	-0.5595369981
28	C	-4.0774263942	1.6572622757	-0.5593734148
29	C	-3.3173422048	2.6521112136	-1.2821742113
30	C	-2.0877073207	2.0373058646	-1.7294714939
31	C	1.8345326715	1.4122471505	1.0218644066
32	C	1.8373240725	2.7882890218	0.5748172021
33	C	1.8391131366	3.6376018909	1.7456785783
34	C	1.8383809926	2.7876846728	2.9161823645
35	C	1.8356185448	1.4117351124	2.4694382533
36	C	-2.0887323026	-1.0139683877	1.0223389258
37	C	-2.0882095077	-1.0140057262	2.4688904552
38	C	-3.3178493314	-0.3987043200	2.9157297777
39	C	-4.0780020838	-0.0187048096	1.7461604592
40	C	-3.3184930501	-0.3984150862	0.5760680187
41	C	-4.8138263373	2.0258292442	2.9161694537
42	C	-4.8137025166	3.4008222983	2.4695456458
43	C	-4.8139839666	3.4010043415	1.0238434733
44	C	-4.8143361753	2.0261265471	0.5768496997
45	C	-4.8143092244	1.1761676774	1.7464131560
46	C	-0.8918775170	5.8248300620	1.0233821102
47	C	-0.8915198486	5.8247083730	2.4690287611
48	C	0.3381558369	5.2095946674	2.9157775841
49	C	1.0982594196	4.8301859563	1.7457284726
50	C	0.3376233775	5.2098510839	0.5759599416
51	C	-4.0760313037	4.3669738419	0.3219662519
52	C	-3.3156382434	5.3616367759	1.0447683575
53	C	-2.0859246345	5.5963914546	0.3217660282
54	C	-2.0864217284	4.7468228845	-0.8480870291
55	C	-3.3163713246	3.9868623385	-0.8478489628
56	C	-2.0852066642	4.7460706642	4.3405954714
57	C	-2.0852609410	5.5959939823	3.1710045086
58	C	-3.3152906320	5.3614231137	2.4484438308
59	C	-4.0753946341	4.3665874124	3.1713495910
60	C	-3.3151781884	3.9861886976	4.3407255779
61	H	-0.6222798669	1.8108109674	1.6525697287
62	F	-1.3857731338	2.3331648879	1.7346103038

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DF-LMP2/VTZ optimized structure of CO@C60 (C5v)

1	C	0.8902484812	0.0649427515	-0.8466766192
2	C	-0.3400446614	0.8253057297	-0.8466766192
3	C	-1.1004076396	0.4451242406	0.3234016910
4	C	-0.3400446614	-0.5502038198	1.0465498562
5	C	0.8902484812	-0.7851689020	0.3234016910
6	C	0.8902484812	0.0649427515	4.3444244208
7	C	0.8902484812	-0.7851689020	3.1743461106
8	C	-0.3400446614	-0.5502038198	2.4511979454
9	C	-1.1004076396	0.4451242406	3.1743461106
10	C	-0.3400446614	0.8253057297	4.3444244208
11	C	0.8902484812	2.7763520193	-1.7276668948
12	C	0.8902484812	4.1518615689	-1.2807367498

13	C	-0.3400446614	4.3868266510	-0.5575885846
14	C	-1.1004076396	3.1565335084	-0.5575885846
15	C	-0.3400446614	2.1612054480	-1.2807367498
16	C	0.8902484812	2.7763520193	5.2254146965
17	C	-0.3400446614	2.1612054480	4.7784845515
18	C	-1.1004076396	3.1565335084	4.0553363863
19	C	-0.3400446614	4.3868266510	4.0553363863
20	C	0.8902484812	4.1518615689	4.7784845515
21	C	2.0851135137	2.0378848173	5.2254146965
22	C	3.3154066563	2.6530313886	4.7784845515
23	C	4.0757696345	1.6577033281	4.0553363863
24	C	3.3154066563	0.4274101856	4.0553363863
25	C	2.0851135137	0.6623752677	4.7784845515
26	C	2.0851135137	0.6623752677	-1.2807367498
27	C	3.3154066563	0.4274101856	-0.5575885846
28	C	4.0757696345	1.6577033281	-0.5575885846
29	C	3.3154066563	2.6530313886	-1.2807367498
30	C	2.0851135137	2.0378848173	-1.7276668948
31	C	-1.8388748417	1.4117903579	1.0257257356
32	C	-1.8388748417	2.7872999074	0.5787955906
33	C	-1.8388748417	3.6374115609	1.7488739008
34	C	-1.8388748417	2.7872999074	2.9189522110
35	C	-1.8388748417	1.4117903579	2.4720220660
36	C	2.0851135137	-1.0133678172	1.0257257356
37	C	2.0851135137	-1.0133678172	2.4720220660
38	C	3.3154066563	-0.3982212459	2.9189522110
39	C	4.0757696345	-0.0180397568	1.7488739008
40	C	3.3154066563	-0.3982212459	0.5787955906
41	C	4.8142368366	2.0269369292	2.9189522110
42	C	4.8142368366	3.4024464787	2.4720220660
43	C	4.8142368366	3.4024464787	1.0257257356
44	C	4.8142368366	2.0269369292	0.5787955906
45	C	4.8142368366	1.1768252757	1.7488739008
46	C	0.8902484812	5.8276046538	1.0257257356
47	C	0.8902484812	5.8276046538	2.4720220660
48	C	-0.3400446614	5.2124580825	2.9189522110
49	C	-1.1004076396	4.8322765934	1.7488739008
50	C	-0.3400446614	5.2124580825	0.5787955906
51	C	4.0757696345	4.3691125960	0.3234016910
52	C	3.3154066563	5.3644406564	1.0465498562
53	C	2.0851135137	5.5994057386	0.3234016910
54	C	2.0851135137	4.7492940851	-0.8466766192
55	C	3.3154066563	3.9889311069	-0.8466766192
56	C	2.0851135137	4.7492940851	4.3444244208
57	C	2.0851135137	5.5994057386	3.1743461106
58	C	3.3154066563	5.3644406564	2.4511979454
59	C	4.0757696345	4.3691125960	3.1743461106
60	C	3.3154066563	3.9889311069	4.3444244208
61	C	1.2676385680	2.0510822885	1.4901985111
62	O	1.7783526193	2.8774349819	2.0905788860

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DF-LMP2/VTZ optimized structure of LiH@C60 (C5v)

1	C	-0.8900729731	0.0649299483	-0.8465097011
2	C	0.3399776233	0.8251430248	-0.8465097011
3	C	1.1001906997	0.4450364866	0.3233379340
4	C	0.3399776233	-0.5500953499	1.0463435341
5	C	-0.8900729731	-0.7850141098	0.3233379340

6	C	-0.8900729731	0.0649299483	4.3438763646
7	C	-0.8900729731	-0.7850141098	3.1740287295
8	C	0.3399776233	-0.5500953499	2.4510231294
9	C	1.1001906997	0.4450364866	3.1740287295
10	C	0.3399776233	0.8251430248	4.3438763646
11	C	-0.8900729731	2.7760980054	-1.7274216026
12	C	-0.8900729731	4.1513363800	-1.2805795677
13	C	0.3399776233	4.3862551400	-0.5575739675
14	C	1.1001906997	3.1562045436	-0.5575739675
15	C	0.3399776233	2.1610727072	-1.2805795677
16	C	-0.8900729731	2.7760980054	5.2247882661
17	C	0.3399776233	2.1610727072	4.7779462312
18	C	1.1001906997	3.1562045436	4.0549406311
19	C	0.3399776233	4.3862551400	4.0549406311
20	C	-0.8900729731	4.1513363800	4.7779462312
21	C	-2.0849648063	2.0376142396	5.2247882661
22	C	-3.3150154027	2.6526395378	4.7779462312
23	C	-4.0752284792	1.6575077014	4.0549406311
24	C	-3.3150154027	0.4274571050	4.0549406311
25	C	-2.0849648063	0.6623758649	4.7779462312
26	C	-2.0849648063	0.6623758649	-1.2805795677
27	C	-3.3150154027	0.4274571050	-0.5575739675
28	C	-4.0752284792	1.6575077014	-0.5575739675
29	C	-3.3150154027	2.6526395378	-1.2805795677
30	C	-2.0849648063	2.0376142396	-1.7274216026
31	C	1.8386744655	1.4117242861	1.0256777316
32	C	1.8386744655	2.7869626607	0.5788356967
33	C	1.8386744655	3.6369067189	1.7486833318
34	C	1.8386744655	2.7869626607	2.9185309668
35	C	1.8386744655	1.4117242861	2.4716889319
36	C	-2.0849648063	-1.0132181435	1.0256777316
37	C	-2.0849648063	-1.0132181435	2.4716889319
38	C	-3.3150154027	-0.3981928453	2.9185309668
39	C	-4.0752284792	-0.0180863071	1.7486833318
40	C	-3.3150154027	-0.3981928453	0.5788356967
41	C	-4.8137122449	2.0267495842	2.9185309668
42	C	-4.8137122449	3.4019879589	2.4716889319
43	C	-4.8137122449	3.4019879589	1.0256777316
44	C	-4.8137122449	2.0267495842	0.5788356967
45	C	-4.8137122449	1.1768055261	1.7486833318
46	C	-0.8900729731	5.8269303885	1.0256777316
47	C	-0.8900729731	5.8269303885	2.4716889319
48	C	0.3399776233	5.2119050903	2.9185309668
49	C	1.1001906997	4.8317985520	1.7486833318
50	C	0.3399776233	5.2119050903	0.5788356967
51	C	-4.0752284792	4.3686757584	0.3233379340
52	C	-3.3150154027	5.3638075948	1.0463435341
53	C	-2.0849648063	5.5987263548	0.3233379340
54	C	-2.0849648063	4.7487822966	-0.8465097011
55	C	-3.3150154027	3.9885692202	-0.8465097011
56	C	-2.0849648063	4.7487822966	4.3438763646
57	C	-2.0849648063	5.5987263548	3.1740287295
58	C	-3.3150154027	5.3638075948	2.4510231294
59	C	-4.0752284792	4.3686757584	3.1740287295
60	C	-3.3150154027	3.9885692202	4.3438763646
61	Li	-0.9525140512	1.5412001096	1.1197474238
62	H	-1.6919280282	2.7375970562	1.9889806858

DF-LMP2/VTZ optimized structure of LiF@C60 (C5v)

1	C	-0.8900545762	0.0649286063	-0.8464922046
2	C	0.3399705963	0.8251259699	-0.8464922046
3	C	1.1001679599	0.4450272881	0.3233312509
4	C	0.3399705963	-0.5500839799	1.0463219073
5	C	-0.8900545762	-0.7849978844	0.3233312509
6	C	-0.8900545762	0.0649286063	4.3434991969
7	C	-0.8900545762	-0.7849978844	3.1736757414
8	C	0.3399705963	-0.5500839799	2.4506850851
9	C	1.1001679599	0.4450272881	3.1736757414
10	C	0.3399705963	0.8251259699	4.3434991969
11	C	-0.8900545762	2.7757673076	-1.7272970919
12	C	-0.8900545762	4.1509772575	-1.2804642928
13	C	0.3399705963	4.3858911619	-0.5574736364
14	C	1.1001679599	3.1558659894	-0.5574736364
15	C	0.3399705963	2.1607547214	-1.2804642928
16	C	-0.8900545762	2.7757673076	5.2243040843
17	C	0.3399705963	2.1607547214	4.7774712851
18	C	1.1001679599	3.1558659894	4.0544806288
19	C	0.3399705963	4.3858911619	4.0544806288
20	C	-0.8900545762	4.1509772575	4.7774712851
21	C	-2.0846772486	2.0374498924	5.2243040843
22	C	-3.3147024211	2.6524624786	4.7774712851
23	C	-4.0748997847	1.6573512106	4.0544806288
24	C	-3.3147024211	0.4273260381	4.0544806288
25	C	-2.0846772486	0.6622399425	4.7774712851
26	C	-2.0846772486	0.6622399425	-1.2804642928
27	C	-3.3147024211	0.4273260381	-0.5574736364
28	C	-4.0748997847	1.6573512106	-0.5574736364
29	C	-3.3147024211	2.6524624786	-1.2804642928
30	C	-2.0846772486	2.0374498924	-1.7272970919
31	C	1.8384853752	1.4114973319	1.0255128398
32	C	1.8384853752	2.7867072818	0.5786800407
33	C	1.8384853752	3.6366337725	1.7485034962
34	C	1.8384853752	2.7867072818	2.9183269517
35	C	1.8384853752	1.4114973319	2.4714941525
36	C	-2.0846772486	-1.0131505129	1.0255128398
37	C	-2.0846772486	-1.0131505129	2.4714941525
38	C	-3.3147024211	-0.3981379267	2.9183269517
39	C	-4.0748997847	-0.0180392449	1.7485034962
40	C	-3.3147024211	-0.3981379267	0.5786800407
41	C	-4.8132172000	2.0265099182	2.9183269517
42	C	-4.8132172000	3.4017198680	2.4714941525
43	C	-4.8132172000	3.4017198680	1.0255128398
44	C	-4.8132172000	2.0265099182	0.5786800407
45	C	-4.8132172000	1.1765834275	1.7485034962
46	C	-0.8900545762	5.8263677129	1.0255128398
47	C	-0.8900545762	5.8263677129	2.4714941525
48	C	0.3399705963	5.2113551267	2.9183269517
49	C	1.1001679599	4.8312564449	1.7485034962
50	C	0.3399705963	5.2113551267	0.5786800407
51	C	-4.0748997847	4.3681899119	0.3233312509
52	C	-3.3147024211	5.3633011799	1.0463219073
53	C	-2.0846772486	5.5982150844	0.3233312509
54	C	-2.0846772486	4.7482885937	-0.8464922046
55	C	-3.3147024211	3.9880912301	-0.8464922046
56	C	-2.0846772486	4.7482885937	4.3434991969
57	C	-2.0846772486	5.5982150844	3.1736757414

58	C	-3.3147024211	5.3633011799	2.4506850851
59	C	-4.0748997847	4.3681899119	3.1736757414
60	C	-3.3147024211	3.9880912301	4.3434991969
61	Li	-0.9557814468	1.5464868668	1.1235884777
62	F	-1.6911490548	2.7363366508	1.9880649477

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DF-LMP2/VTZ optimized structure of BN@C60 (C2v)

1	C	-0.8890400849	0.0532344128	-0.8993450137
2	C	0.3499749320	0.8189864043	-0.8993467602
3	C	1.1100669443	0.4816040770	0.2803521295
4	C	0.2656703523	-0.4298605166	1.0298652205
5	C	-0.9271982475	-0.7774918425	0.2803535032
6	C	-0.8866311262	0.0493408708	4.3790262032
7	C	-0.9258520836	-0.7796645129	3.1981566315
8	C	0.2663434304	-0.4309546040	2.4480984652
9	C	1.1114057839	0.4794321787	3.1981549717
10	C	0.3523819782	0.8150939542	4.3790252175
11	C	-0.8925727462	2.7799488477	-1.7413347372
12	C	-0.8910113547	4.1507721971	-1.2869775315
13	C	0.3347977625	4.3782847800	-0.5582499331
14	C	1.0934609447	3.1500904912	-0.5580631651
15	C	0.3367968945	2.1640027361	-1.2992625333
16	C	-0.8893989205	2.7748150837	5.2250398950
17	C	0.3395656840	2.1595195565	4.7809279010
18	C	1.0955614272	3.1467042156	4.0405132882
19	C	0.3368957698	4.3748945409	4.0432021874
20	C	-0.8882498158	4.1463063278	4.7727085849
21	C	-2.0841181364	2.0364374096	5.2250411495
22	C	-3.3113314530	2.6487585772	4.7727105482
23	C	-4.0636875183	1.6551833015	4.0432029374
24	C	-3.3044471414	0.4273483146	4.0405164185
25	C	-2.0833894929	0.6620503021	4.7809299131
26	C	-2.0861678219	0.6665275641	-1.2992617157
27	C	-3.3065419909	0.4307390755	-0.5580625149
28	C	-4.0657889765	1.6585733189	-0.5582512958
29	C	-3.3140949401	2.6532247617	-1.2869766253
30	C	-2.0872953076	2.0415698687	-1.7413346528
31	C	1.8748697489	1.4191033318	1.0094538263
32	C	1.8556658791	2.7918248009	0.5695075424
33	C	1.8497048859	3.6382723363	1.7412422885
34	C	1.8567203563	2.7900932279	2.9117178297
35	C	1.8755336912	1.4180159184	2.4697414645
36	C	-2.1077513239	-1.0422876406	1.0094557843
37	C	-2.1070761712	-1.0433726999	2.4697427332
38	C	-3.3258867657	-0.4129371262	2.9117210678
39	C	-4.0813836142	-0.0273422707	1.7412449306
40	C	-3.3269633473	-0.4112133476	0.5695107608
41	C	-4.8049760149	2.0227491752	2.9112224092
42	C	-4.8066146612	3.3964464682	2.4662293320
43	C	-4.8072725756	3.3975091323	1.0219667909
44	C	-4.8060382303	2.0244684098	0.5749500542
45	C	-4.8042025620	1.1741440936	1.7424602089
46	C	-0.8889490093	5.8191686965	1.0219670271
47	C	-0.8882924596	5.8181015693	2.4662297846
48	C	0.3396482391	5.2023006578	2.9112209654
49	C	1.0983170174	4.8221021306	1.7424580503
50	C	0.3385833031	5.2040218292	0.5749490319

51	C	-4.0704504415	4.3637627212	0.3213448018
52	C	-3.3114211364	5.3579906431	1.0435924963
53	C	-2.0827088803	5.5922543438	0.3213441753
54	C	-2.0829924546	4.7441658836	-0.8478089837
55	C	-3.3117708160	3.9847392719	-0.8478080197
56	C	-2.0806315348	4.7403465730	4.3355024055
57	C	-2.0814142500	5.5901620925	3.1676046670
58	C	-3.3107820713	5.3569555413	2.4461300599
59	C	-4.0691569083	4.3616680973	3.1676048493
60	C	-3.3094087553	3.9809193554	4.3355028688
61	B	-0.6478300406	1.0482089635	1.7402566100
62	N	-1.3326078088	2.1562377017	1.7416655702

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DF-LMP2/VTZ optimized structure of BeO@C60 (C5v)

1	C	-0.8896730040	0.0649007710	-0.8461293078
2	C	0.3398248486	0.8247722330	-0.8461293078
3	C	1.0996963106	0.4448365020	0.3231926367
4	C	0.3398248486	-0.5498481553	1.0458733422
5	C	-0.8896730040	-0.7846613506	0.3231926367
6	C	-0.8896730040	0.0649007710	4.3424761985
7	C	-0.8896730040	-0.7846613506	3.1731542541
8	C	0.3398248486	-0.5498481553	2.4504735486
9	C	1.0996963106	0.4448365020	3.1731542541
10	C	0.3398248486	0.8247722330	4.3424761985
11	C	-0.8896730040	2.7753753384	-1.7268158809
12	C	-0.8896730040	4.1499957267	-1.2801746419
13	C	0.3398248486	4.3848089220	-0.5574939364
14	C	1.0996963106	3.1553110694	-0.5574939364
15	C	0.3398248486	2.1606264121	-1.2801746419
16	C	-0.8896730040	2.7753753384	5.2231627716
17	C	0.3398248486	2.1606264121	4.7765215326
18	C	1.0996963106	3.1553110694	4.0538408271
19	C	0.3398248486	4.3848089220	4.0538408271
20	C	-0.8896730040	4.1499957267	4.7765215326
21	C	-2.0844973049	2.0369333098	5.2231627716
22	C	-3.3139951575	2.6516822361	4.7765215326
23	C	-4.0738666195	1.6569975788	4.0538408271
24	C	-3.3139951575	0.4274997262	4.0538408271
25	C	-2.0844973049	0.6623129215	4.7765215326
26	C	-2.0844973049	0.6623129215	-1.2801746419
27	C	-3.3139951575	0.4274997262	-0.5574939364
28	C	-4.0738666195	1.6569975788	-0.5574939364
29	C	-3.3139951575	2.6516822361	-1.2801746419
30	C	-2.0844973049	2.0369333098	-1.7268158809
31	C	1.8381383392	1.4114696668	1.0254927399
32	C	1.8381383392	2.7860900551	0.5788515009
33	C	1.8381383392	3.6356521767	1.7481734454
34	C	1.8381383392	2.7860900551	2.9174953899
35	C	1.8381383392	1.4114696668	2.4708541509
36	C	-2.0844973049	-1.0128524868	1.0254927399
37	C	-2.0844973049	-1.0128524868	2.4708541509
38	C	-3.3139951575	-0.3981035605	2.9174953899
39	C	-4.0738666195	-0.0181678295	1.7481734454
40	C	-3.3139951575	-0.3981035605	0.5788515009
41	C	-4.8123086481	2.0262185931	2.9174953899
42	C	-4.8123086481	3.4008389814	2.4708541509
43	C	-4.8123086481	3.4008389814	1.0254927399

44	C	-4.8123086481	2.0262185931	0.5788515009
45	C	-4.8123086481	1.1766564715	1.7481734454
46	C	-0.8896730040	5.8251611349	1.0254927399
47	C	-0.8896730040	5.8251611349	2.4708541509
48	C	0.3398248486	5.2104122086	2.9174953899
49	C	1.0996963106	4.8304764776	1.7481734454
50	C	0.3398248486	5.2104122086	0.5788515009
51	C	-4.0738666195	4.3674721461	0.3231926367
52	C	-3.3139951575	5.3621568034	1.0458733422
53	C	-2.0844973049	5.5969699987	0.3231926367
54	C	-2.0844973049	4.7474078771	-0.8461293078
55	C	-3.3139951575	3.9875364151	-0.8461293078
56	C	-2.0844973049	4.7474078771	4.3424761985
57	C	-2.0844973049	5.5969699987	3.1731542541
58	C	-3.3139951575	5.3621568034	2.4504735486
59	C	-4.0738666195	4.3674721461	3.1731542541
60	C	-3.3139951575	3.9875364151	4.3424761985
61	Be	-0.7964949868	1.2887559605	0.9363360135
62	O	-1.4128854565	2.2860966908	1.6609464690
