Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for:

Reactivity of the superhalogen/superalkali ion encapsulated C_{60} fullerenes

Gibu George,[a] Anton J. Stasyuk *[ab] and Miquel Solà *[a]

a. Institut de Química Computacional and Departament de Química, Universitat de Girona, C/ Maria Aurèlia Capmany 69, 17003 Girona, Catalonia, Spain.
b. Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland.

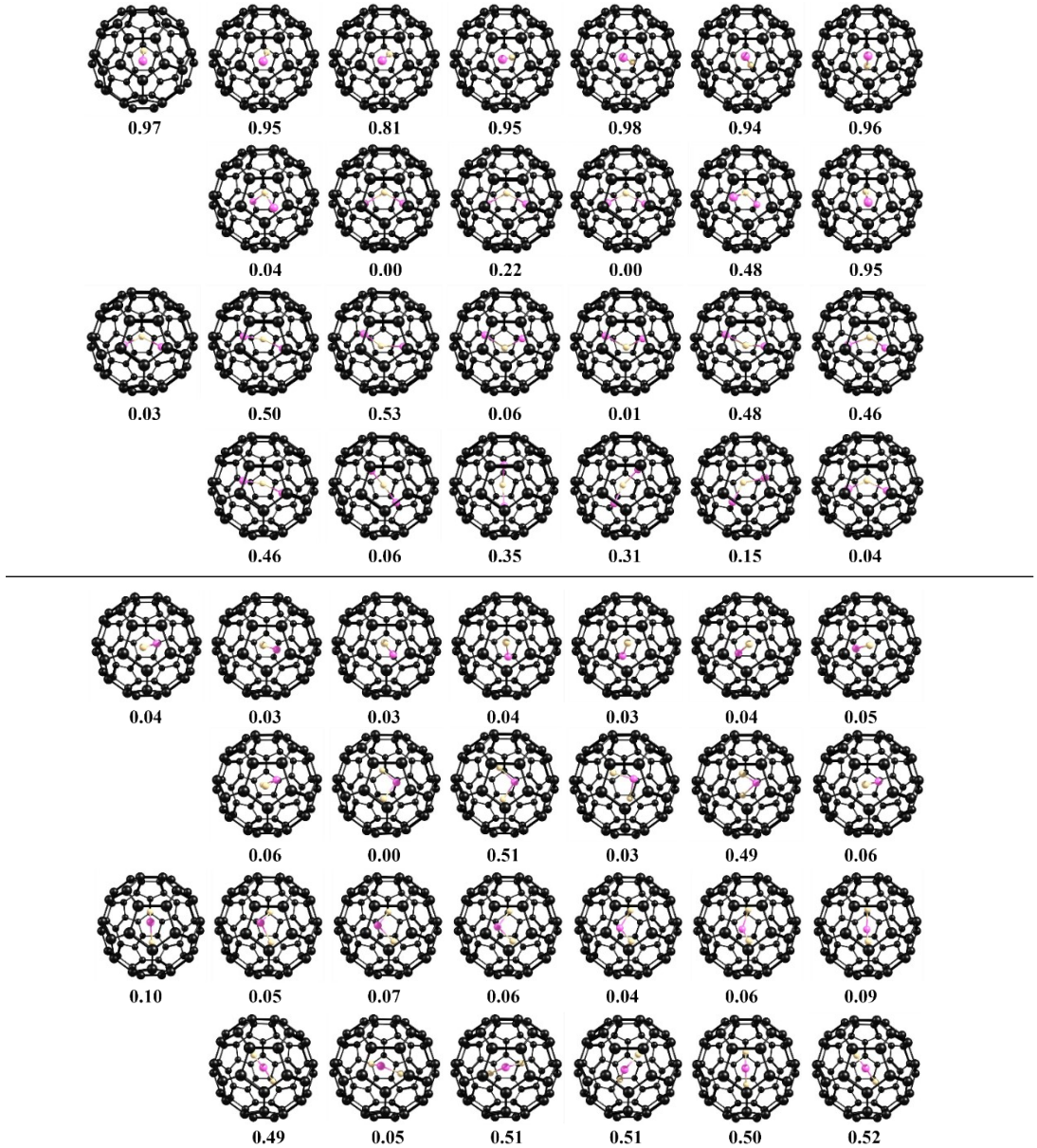

Figure S1. Structures of $Li_2F^+@C_{60}$ and $LiF_2^-@C_{60}$, where Li_2F^+ and LiF_2^- fragments are inside the fullerene cage in different orientations. Relative energy values are given in kcal/mol. Black-, pink-, and yellow-colored balls represent carbon, lithium and fluorine atoms.

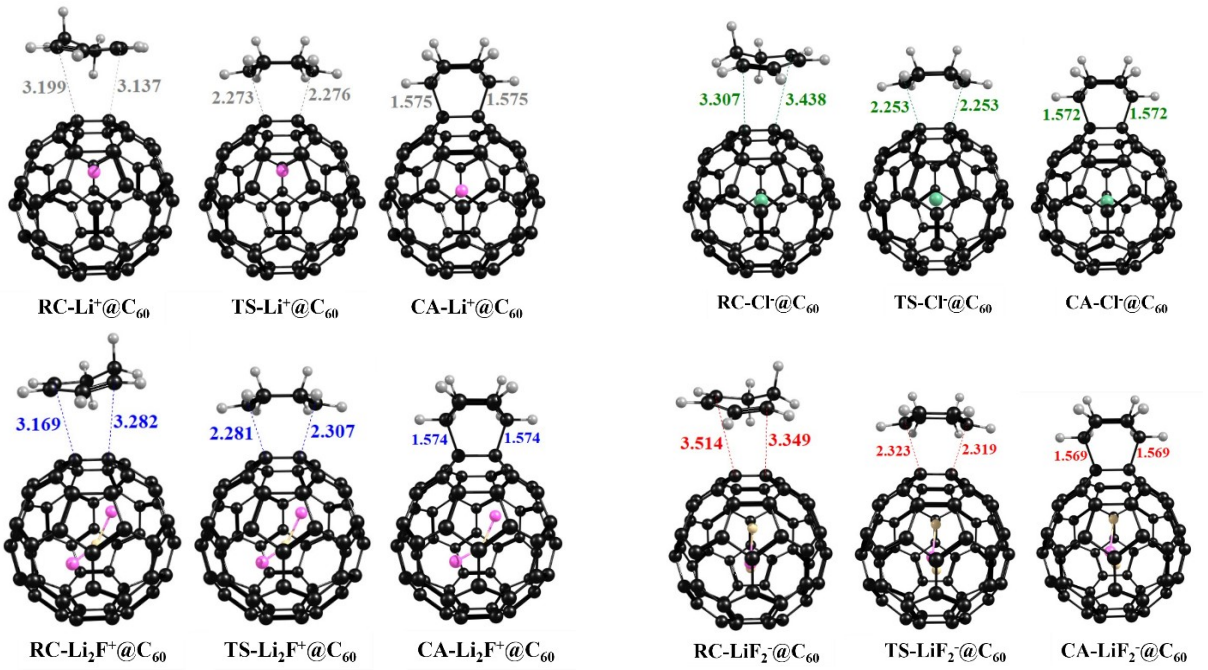

Figure S2. Structures of the RC, CA, and the transition states involved in the Diels-Alder reaction between 1,3-CHD and the encapsulated cationic/anionic species were obtained at M06-2X-D3/def2-SVP level of theory. Highlighted bond lengths are given in angstroms.

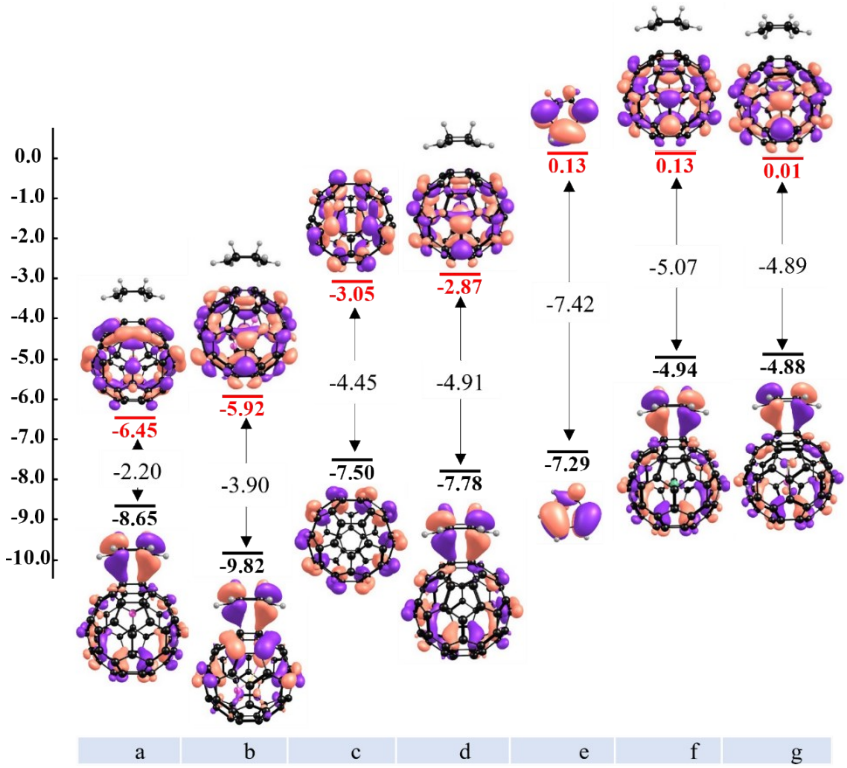

Figure S3. Frontier HOMO and LUMO of (a) TS-Li^+@C_{60}, (b) TS-Li_2F^+@C_{60}, (c) isolated C_{60}, (d) TS-C_{60}, (e) isolated 1,3-CHD, (f) TS-Cl^-@C_{60}, (g) TS-LiF_2^-@C_{60} with energies in eV computed at M06-2X-D3/def2-TZVPP//M06-2X-D3/def2-SVP level of theory. Orbitals are drawn on the isodensity surface of 0.03 e/Å^3.

Table S1. ASM results for the Diels-Alder reaction between 1,3-CHD and Li_2F^+@C60 along the intrinsic reaction coordinate projected onto the forming C···C bond length. The energies were computed at M06-2X-D3/def2-TZVPP//M06-2X-D3/def2-SVP level of theory. Energies are given in kcal/mol.

C···C distance (Å)	ΔE_{int}	ΔE_{strain}	ΔE
TS-Li_2F^+@C_{60} (2.3 Å)	-18.66	23.98	5.32
2.4 Å	-11.02	14.92	3.90
2.5 Å	-7.39	9.34	1.95
2.6 Å	-6.27	6.34	0.06
2.7 Å	-6.32	4.37	-1.94
2.8 Å	-6.98	3.65	-3.32
2.9 Å	-7.91	3.20	-4.71
3.0 Å	-8.56	3.00	-5.56
RC-Li_2F^+@C_{60} (3.1 Å)	-8.57	0.56	-8.01

Table S2. ASM results for the Diels-Alder reaction between 1,3-CHD and C_{60} along the intrinsic reaction coordinate projected onto the forming C···C bond length. The energies were computed at M06-2X-D3/def2-TZVPP//M06-2X-D3/def2-SVP level of theory. Energies are given in kcal/mol.

C···C distance (Å)	ΔE_{int}	ΔE_{strain}	ΔE
TS-C_{60} (2.3 Å)	-13.09	25.34	12.24
2.4 Å	-4.67	15.09	10.42
2.5 Å	-1.44	9.15	7.70
2.6 Å	-0.90	5.95	5.05
2.7 Å	-1.50	4.44	2.94
2.8 Å	-2.87	3.37	0.49
2.9 Å	-4.12	2.97	-1.14
3.0 Å	-5.30	2.74	-2.55
RC-C_{60} (3.3 Å)	-6.17	0.47	-5.69

Table S3. ASM results for the Diels-Alder reaction between 1,3-CHD and $LiF_2^-@C_{60}$ along the intrinsic reaction coordinate projected onto the forming C···C bond length. The energies were computed at M06-2X-D3/def2-TZVPP//M06-2X-D3/def2-SVP level of theory. Energies are given in kcal/mol.

C···C distance (Å)	ΔE_{int}	ΔE_{strain}	ΔE
TS-$LiF_2^-@C_{60}$ (2.3 Å)	-8.85	21.57	12.72
2.4 Å	-3.63	15.34	11.70
2.5 Å	-0.17	9.57	9.40
2.6 Å	0.42	6.53	6.96
2.7 Å	-0.07	4.98	4.91
2.8 Å	-1.43	3.73	2.30
2.9 Å	-2.71	3.23	0.51
3.0 Å	-4.04	2.91	-1.13
RC-$LiF_2^-@C_{60}$ (3.5 Å)	-5.36	0.41	-4.95

Table S4. EDA results for the Diels-Alder reaction between 1,3-CHD and $Li_2F^+@C_{60}$ along the intrinsic reaction coordinate projected onto the forming C···C bond length. The energies were computed at B3LYP-D3/TZ2P//M06-2X-D3/def2-SVP level of theory.[a,b]

C···C distance (Å)	Energy terms				
	ΔE_{pauli}	ΔV_{elstat}	ΔE_{orb}	ΔE_{disp}	ΔE_{int}
TS-$Li_2F^+@C_{60}$ (2.3 Å)	100.23	-47.46 (40.5%)	-57.06 (48.6%)	-12.77 (10.9%)	-17.06
2.4 Å	80.25	-37.62 (41.5%)	-40.23 (44.3%)	-12.85 (14.2%)	-10.44
2.5 Å	65.50	-30.53 (41.9%)	-29.59 (40.6%)	-12.72 (17.5%)	-7.34
2.6 Å	54.62	-25.43 (41.8%)	-22.93 (37.7%)	-12.50 (20.5%)	-6.24
2.7 Å	44.35	-20.76 (41.1%)	-17.77 (35.1%)	-12.04 (23.8%)	-6.22
2.8 Å	36.98	-17.48 (39.8%)	-14.82 (33.7%)	-11.65 (26.5%)	-6.97
2.9 Å	28.58	-13.81 (37.7%)	-11.85 (32.4%)	-10.96 (29.9%)	-8.04
3.0 Å	21.20	-10.59 (35.2%)	-9.33 (31.1%)	-10.12 (33.7%)	-8.84
RC-$Li_2F^+@C_{60}$ (3.1 Å)	16.35	-8.63 (35.4%)	-6.45 (26.4%)	-9.30 (18.2%)	-8.02

[a] The energy values are in kcal/mol. [b] The percentage contributions to the sum of all attractive energy terms are given in parentheses.

Table S5. EDA results for the Diels-Alder reaction between 1,3-CHD and C_{60} along the intrinsic reaction coordinate projected onto the forming C···C bond length. The energies were computed at B3LYP-D3/TZ2P//M06-2X-D3/def2-SVP level of theory.[a,b]

C···C distance (Å)	Energy terms				
	ΔE_{pauli}	ΔV_{elstat}	ΔE_{orb}	ΔE_{disp}	ΔE_{int}
TS-C_{60} (2.3 Å)	109.15	-51.97 (43.2%)	-54.98 (45.8%)	-13.20 (11.0%)	-11.00
2.4 Å	86.05	-40.36 (45.0%)	-35.96 (40.1%)	-13.31 (14.8%)	-3.59
2.5 Å	69.20	-32.09 (45.9%)	-24.60 (35.2%)	-13.25 (18.9%)	-0.73
2.6 Å	57.01	-26.22 (45.8%)	-17.92 (31.3%)	-13.04 (22.8%)	-0.17
2.7 Å	48.18	-22.13 (45.3%)	-14.00 (28.6%)	-12.74 (26.1%)	-0.70
2.8 Å	37.83	-17.40 (43.5%)	-10.42 (26.1%)	-12.17 (30.4%)	-2.16
2.9 Å	30.31	-14.01 (41.4%)	-8.28 (24.5%)	-11.56 (34.1%)	-3.54
3.0 Å	22.27	-10.40 (38.2%)	-6.16 (22.6%)	-10.69 (39.2%)	-4.98
RC-C_{60} (3.3 Å)	14.11	-6.80 (35.0%)	-3.38 (17.4%)	-9.27(47.7%)	-5.35

[a] The energy values are in kcal/mol. [b] The percentage contributions to the sum of all attractive energy terms are given in parentheses.

Table S6. EDA results for the Diels-Alder reaction between 1,3-CHD and $LiF_2^-@C_{60}$ along the intrinsic reaction coordinate projected onto the forming C···C bond length. The energies were computed at B3LYP-D3/TZ2P//M06-2X-D3/def2-SVP level of theory.[a,b]

C···C distance (Å)	Energy terms				
	ΔE_{pauli}	ΔV_{elstat}	ΔE_{orb}	ΔE_{disp}	ΔE_{int}
TS-$LiF_2^-@C_{60}$ (2.3 Å)	100.85	-48.30 (44.8%)	-46.47 (43.1%)	-13.09 (12.1%)	-7.01
2.4 Å	86.65	-41.05 (46.1%)	-34.81 (39.1%)	-13.14 (14.8%)	-2.35
2.5 Å	70.38	-32.91 (47.3%)	-23.61 (33.9%)	-13.05 (18.8%)	0.80
2.6 Å	58.60	-27.03 (47.4%)	-17.14 (30.1%)	-12.84 (22.5%)	1.60
2.7 Å	50.13	-22.85 (46.8%)	-13.45 (27.5%)	-12.54 (25.7%)	1.30
2.8 Å	39.54	-17.83 (45.1%)	-9.78 (24.7%)	-11.96 (30.2%)	-0.04
2.9 Å	31.85	-14.26 (42.8%)	-7.69 (23.1%)	-11.36 (34.1%)	-1.46
3.0 Å	23.46	-10.36 (39.1%)	-5.66 (21.3%)	-10.49 (39.6%)	-3.04
RC-$LiF_2^-@C_{60}$ (3.5 Å)	13.37	-5.96 (33.7%)	-3.03 (17.1%)	-8.70 (49.2%)	-4.31

[a] The energy values are in kcal/mol. [b] The percentage contributions to the sum of all attractive energy terms are given in parentheses.

Cartesian coordinates (in Å) and electronic energies (in a.u.) of all the stationary points discussed in the text. All calculations have been performed at the M06-2X-D3/def2-TZVPP//M06-2X-D3/def2-SVP level.

1,3-cyclohexadiene: E = -233.3933694

C	-0.31475000	0.69680000	-1.18854000
C	-0.05286000	1.42083000	0.10828000
C	0.31475000	-0.69680000	-1.18854000
H	-0.01074000	2.51260000	0.11031000
H	-0.05093000	-1.28127000	-2.04440000
C	0.05286000	0.73314000	1.25495000
C	0.05286000	-1.42083000	0.10828000
H	0.19521000	1.25234000	2.20481000
H	0.01074000	-2.51260000	0.11031000
C	-0.05286000	-0.73314000	1.25495000
H	-0.19521000	-1.25234000	2.20481000
H	-1.41041000	0.60779000	-1.31891000
H	0.05093000	1.28127000	-2.04440000
H	1.41041000	-0.60779000	-1.31891000

C_{60}: E = -2286.1854507

C	-0.72612000	3.41706000	0.59120000
C	-1.17503000	2.79971000	1.82681000
C	0.00000000	2.41798000	2.59048000
C	1.17503000	2.79971000	1.82681000
C	0.72612000	3.41706000	0.59120000
C	3.47420000	0.36535000	0.59120000
C	3.02543000	1.74651000	0.59120000
C	2.29958000	1.98267000	1.82681000
C	2.29964000	0.74720000	2.59048000
C	3.02578000	-0.25236000	1.82681000
C	-3.02543000	1.74651000	0.59120000
C	-3.47420000	0.36535000	0.59120000
C	-3.02578000	-0.25236000	1.82681000
C	-2.29964000	0.74720000	2.59048000
C	-2.29958000	1.98267000	1.82681000
C	2.59594000	-2.33765000	0.59120000
C	2.59624000	-1.57435000	1.82681000
C	1.42125000	-1.95619000	2.59048000
C	0.69501000	-2.95567000	1.82681000
C	1.42105000	-3.19126000	0.59120000
C	3.02543000	-1.74651000	-0.59120000
C	2.29958000	-1.98267000	-1.82681000
C	2.29964000	-0.74720000	-2.59048000
C	3.02578000	0.25236000	-1.82681000
C	3.47420000	-0.36535000	-0.59120000
C	-1.42105000	3.19126000	-0.59120000
C	-0.69501000	2.95567000	-1.82681000
C	-1.42125000	1.95619000	-2.59048000
C	-2.59624000	1.57435000	-1.82681000

C	-2.59594000	2.33765000	-0.59120000
C	0.00000000	1.23548000	3.32109000
C	-1.17501000	0.38178000	3.32109000
C	-0.72620000	-0.99952000	3.32109000
C	0.72620000	-0.99952000	3.32109000
C	1.17501000	0.38178000	3.32109000
C	1.42105000	3.19126000	-0.59120000
C	2.59594000	2.33765000	-0.59120000
C	2.59624000	1.57435000	-1.82681000
C	1.42125000	1.95619000	-2.59048000
C	0.69501000	2.95567000	-1.82681000
C	1.17501000	-0.38178000	-3.32109000
C	0.00000000	-1.23548000	-3.32109000
C	-1.17501000	-0.38178000	-3.32109000
C	-0.72620000	0.99952000	-3.32109000
C	0.72620000	0.99952000	-3.32109000
C	-2.59594000	-2.33765000	0.59120000
C	-1.42105000	-3.19126000	0.59120000
C	-0.69501000	-2.95567000	1.82681000
C	-1.42125000	-1.95619000	2.59048000
C	-2.59624000	-1.57435000	1.82681000
C	-2.29964000	-0.74720000	-2.59048000
C	-2.29958000	-1.98267000	-1.82681000
C	-3.02543000	-1.74651000	-0.59120000
C	-3.47420000	-0.36535000	-0.59120000
C	-3.02578000	0.25236000	-1.82681000
C	0.72612000	-3.41706000	-0.59120000
C	-0.72612000	-3.41706000	-0.59120000
C	-1.17503000	-2.79971000	-1.82681000
C	0.00000000	-2.41798000	-2.59048000
C	1.17503000	-2.79971000	-1.82681000

$Li_2F^+@C_{60}$: E = -2401.0500268

C	3.27792900	1.39520900	0.35511000
C	2.42164700	2.47472100	0.83655500
C	1.90698700	2.09861500	2.14358900
C	2.43124500	0.78402700	2.47251300
C	3.27848200	0.34449900	1.37034700
C	0.26658700	-2.03319700	2.87734900
C	1.62299200	-1.53077500	2.74233100
C	1.62546300	-0.13393700	3.13862700
C	0.26950000	0.22445600	3.51824600
C	-0.56980400	-0.94912200	3.35735500
C	1.59575500	2.81326200	-1.46184300
C	0.23322300	2.95384200	-1.94971300
C	-0.59973300	3.39434200	-0.84549900
C	0.24731300	3.52472400	0.32635200
C	1.60470200	3.16652500	-0.05309700
C	-2.39922900	-1.76041900	1.92707500
C	-1.87413100	-0.81545100	2.89601700

C	-2.39777200	0.50129700	2.57187600
C	-3.25826600	0.37394300	1.40139800
C	-3.25328500	-1.02939700	1.00088500
C	-1.59327200	-2.79207500	1.45969400
C	-1.60210900	-3.14700800	0.05227400
C	-0.24704700	-3.50843800	-0.32674100
C	0.59945900	-3.37746700	0.84481000
C	-0.23296400	-2.93430900	1.94801100
C	3.26578600	1.05316300	-1.00288900
C	3.25618600	-0.35158600	-1.40175200
C	2.39828700	-0.48216300	-2.57242400
C	1.87517400	0.83317600	-2.89723500
C	2.40287200	1.78012500	-1.92816800
C	0.60635000	2.43759900	2.50313700
C	-0.23992000	3.16782700	1.57635900
C	-1.59800500	2.66631700	1.71067300
C	-1.59012700	1.62355700	2.72148000
C	-0.22796300	1.48298900	3.20956700
C	3.26549400	-0.99988700	0.98488800
C	2.42298100	-1.95742900	1.68944600
C	1.89876400	-2.90140800	0.71792300
C	2.40921400	-2.52991800	-0.58953300
C	3.25526800	-1.35489300	-0.42899300
C	0.23931900	-3.15175500	-1.57620000
C	-0.60594100	-2.41955400	-2.50072500
C	0.22799200	-1.46308900	-3.20542300
C	1.58871600	-1.60343800	-2.71733800
C	1.59531300	-2.64808900	-1.70917900
C	-2.42985800	1.97779000	-1.69153800
C	-3.28178200	1.02531200	-0.98762700
C	-3.27500200	1.38161700	0.42980700
C	-2.41635400	2.55071200	0.59050400
C	-1.90183700	2.91982800	-0.71841000
C	-0.26910700	-0.20657000	-3.52149300
C	-1.62538400	0.15180600	-3.14168600
C	-1.62488700	1.54800900	-2.74251100
C	-0.26724300	2.04975400	-2.87665000
C	0.57007000	0.96599300	-3.35899600
C	-3.25951900	-1.36947200	-0.35391700
C	-3.27132900	-0.32142000	-1.36835100
C	-2.42728300	-0.76459300	-2.47101400
C	-1.90492000	-2.08031000	-2.14239400
C	-2.41589000	-2.45450100	-0.83625200
F	0.00037200	-0.48286100	0.00276800
Li	-1.51456700	0.13112800	0.00134500
Li	1.51524000	0.13072400	-0.00286500

$LiF_2^-@C_{60}$: E = -2493.5981756

C	-2.41162000	0.61342000	2.52694000
C	-3.29649000	0.38544000	1.39096000

C	-3.27687000	-1.04379000	1.09201000
C	-2.37318000	-1.67706000	2.04449000
C	-1.84682000	-0.65842000	2.93198000
C	0.68082000	-3.27824000	1.06399000
C	-0.16240000	-2.78679000	2.13359000
C	-1.53331000	-2.71231000	1.65258000
C	-1.54226000	-3.16109000	0.27865000
C	-0.17642000	-3.50929000	-0.07997000
C	-2.48569000	2.50219000	0.43056000
C	-1.97485000	2.78698000	-0.89869000
C	-2.49992000	1.77537000	-1.79789000
C	-3.34529000	0.86710000	-1.03264000
C	-3.33417000	1.31864000	0.35522000
C	1.65536000	-2.72234000	-1.52312000
C	0.30519000	-3.23329000	-1.34658000
C	-0.56880000	-2.58856000	-2.30485000
C	0.24718000	-1.67621000	-3.07803000
C	1.61815000	-1.75512000	-2.59720000
C	2.48810000	-2.50841000	-0.43036000
C	3.34115000	-1.32743000	-0.35780000
C	3.34677000	-0.87274000	1.03179000
C	2.49903000	-1.78038000	1.79611000
C	1.97532000	-2.78924000	0.89647000
C	-1.62030000	1.75513000	2.60577000
C	-0.24936000	1.67819000	3.08839000
C	0.56879000	2.59153000	2.31350000
C	-0.30479000	3.23793000	1.35100000
C	-1.65639000	2.72226000	1.52826000
C	-3.28655000	-1.47605000	-0.23419000
C	-3.31766000	-0.49789000	-1.31932000
C	-2.44374000	-0.98672000	-2.37902000
C	-1.87774000	-2.25426000	-1.96185000
C	-2.39019000	-2.55255000	-0.63935000
C	-0.53384000	-0.73120000	3.39485000
C	0.33193000	-1.82064000	2.99125000
C	1.68130000	-1.30778000	2.81689000
C	1.65275000	0.10725000	3.11449000
C	0.28679000	0.45981000	3.47312000
C	3.31971000	0.49164000	1.32215000
C	3.27711000	1.46462000	0.23551000
C	2.38671000	2.54655000	0.63913000
C	1.87765000	2.25012000	1.96520000
C	2.44713000	0.98176000	2.38179000
C	-0.33034000	1.81759000	-2.99301000
C	0.53381000	0.72643000	-3.39804000
C	-0.28870000	-0.46396000	-3.47664000
C	-1.65401000	-0.11335000	-3.11847000
C	-1.68023000	1.30161000	-2.81770000
C	1.54497000	3.16825000	-0.28161000
C	1.53584000	2.71843000	-1.65917000
C	0.16406000	2.79535000	-2.14271000
C	-0.68104000	3.28828000	-1.06991000

C	0.17700000	3.52067000	0.07907000
C	2.41657000	-0.62009000	-2.52960000
C	1.84662000	0.65129000	-2.93333000
C	2.36750000	1.66955000	-2.04287000
C	3.26670000	1.03114000	-1.08941000
C	3.30412000	-0.39557000	-1.39554000
Li	-0.00025000	0.90604000	0.01614000
F	-1.21784000	-0.12570000	-0.00290000
F	1.21714000	-0.12548000	-0.00034000

$Li^{+}@C_{60}$: E = -2293.5120607

C	-1.59921000	-3.00955000	1.00054000
C	-0.23830000	-3.45518000	0.75497000
C	0.59643000	-2.96670000	1.83932000
C	-0.24854000	-2.21780000	2.75392000
C	-1.60560000	-2.24513000	2.23552000
C	0.22194000	1.27924000	3.29954000
C	-0.60792000	0.10312000	3.49634000
C	0.23815000	-1.07135000	3.37165000
C	1.59193000	-0.62147000	3.09649000
C	1.58187000	0.83216000	3.05195000
C	-0.58164000	-3.08612000	-1.65608000
C	0.25218000	-2.38156000	-2.61482000
C	1.60825000	-2.35318000	-2.09417000
C	1.61195000	-3.04153000	-0.81292000
C	0.25816000	-3.49455000	-0.54308000
C	1.86071000	2.66108000	1.42394000
C	2.38593000	1.51039000	2.14025000
C	3.23511000	0.75913000	1.22594000
C	3.23123000	1.44899000	-0.05844000
C	2.37987000	2.62407000	0.06679000
C	0.55485000	3.08198000	1.65380000
C	-0.28613000	3.49155000	0.54190000
C	-1.64089000	3.04311000	0.81491000
C	-1.63721000	2.35574000	2.09440000
C	-0.28015000	2.37894000	2.61292000
C	-2.40085000	-2.61564000	-0.06382000
C	-3.24836000	-1.44219000	0.05902000
C	-3.25201000	-0.75489000	-1.22055000
C	-2.40670000	-1.50315000	-2.13481000
C	-1.88071000	-2.65384000	-1.42010000
C	1.89656000	-2.54276000	1.58356000
C	2.41591000	-2.58196000	0.22647000
C	3.25173000	-1.40535000	0.02913000
C	3.24509000	-0.63793000	1.26883000
C	2.40564000	-1.34312000	2.22766000
C	-2.41318000	-1.12045000	2.35171000
C	-1.90322000	0.07881000	2.99456000
C	-2.42929000	1.22925000	2.27956000
C	-3.26430000	0.74085000	1.19591000

C	-3.25450000	-0.71089000	1.24051000
C	-2.43653000	2.57364000	-0.22299000
C	-1.91637000	2.53573000	-1.57925000
C	-2.42623000	1.33631000	-2.22183000
C	-3.26162000	0.63396000	-1.26317000
C	-3.26792000	1.39841000	-0.02814000
C	1.88343000	-0.07906000	-3.00287000
C	2.39242000	1.12159000	-2.36068000
C	3.23748000	0.71338000	-1.24684000
C	3.24782000	-0.74379000	-1.20217000
C	2.40867000	-1.23095000	-2.28846000
C	-1.62079000	0.62042000	-3.09894000
C	-0.26607000	1.07100000	-3.36857000
C	0.58116000	-0.10299000	-3.49171000
C	-0.24990000	-1.27874000	-3.29642000
C	-1.61079000	-0.83126000	-3.05445000
C	1.57027000	3.00804000	-0.99849000
C	1.57665000	2.24246000	-2.23508000
C	0.22057000	2.22026000	-2.75600000
C	-0.62331000	2.97066000	-1.84185000
C	0.21027000	3.45798000	-0.75632000
Li	1.41201000	0.00168000	0.00195000

Cl^-@C_{60}: E = -2746.5479728

C	2.90962000	0.60832000	1.92230000
C	1.86374000	0.72506000	2.92077000
C	1.36744000	-0.60752000	3.20779000
C	2.10640000	-1.54767000	2.38665000
C	3.05952000	-0.79627000	1.59226000
C	0.49703000	-3.50217000	-0.12386000
C	1.73880000	-3.04687000	0.47205000
C	1.46049000	-2.64853000	1.83875000
C	0.04674000	-2.85802000	2.08752000
C	-0.54866000	-3.38556000	0.87462000
C	1.11347000	2.80633000	1.84709000
C	-0.22083000	3.21905000	1.45536000
C	-1.17395000	2.46769000	2.24996000
C	-0.42856000	1.59061000	3.13270000
C	0.98509000	1.80011000	2.88382000
C	-2.11490000	-2.69471000	-0.89094000
C	-1.82640000	-2.99059000	0.49942000
C	-2.56570000	-2.05070000	1.32053000
C	-3.31084000	-1.17356000	0.43740000
C	-3.03260000	-1.57194000	-0.92943000
C	-1.11349000	-2.80631000	-1.84703000
C	-0.98513000	-1.80006000	-2.88373000
C	0.42852000	-1.59056000	-3.13256000
C	1.17392000	-2.46770000	-2.24993000
C	0.22079000	-3.21902000	-1.45528000

C	3.03253000	1.57197000	0.92948000
C	3.31082000	1.17358000	-0.43734000
C	2.56570000	2.05075000	-1.32049000
C	1.82639000	2.99064000	-0.49937000
C	2.11490000	2.69479000	0.89102000
C	0.01367000	-0.80815000	3.44559000
C	-0.90372000	0.31472000	3.40752000
C	-2.14544000	-0.14081000	2.81196000
C	-1.99543000	-1.54543000	2.48201000
C	-0.66097000	-1.95790000	2.87371000
C	3.32610000	-1.17773000	0.28345000
C	2.65138000	-2.32743000	-0.28883000
C	2.36287000	-2.03164000	-1.67931000
C	2.85902000	-0.69900000	-1.96632000
C	3.45435000	-0.17136000	-0.75334000
C	0.90368000	-0.31470000	-3.40744000
C	-0.01375000	0.80816000	-3.44551000
C	0.66091000	1.95788000	-2.87362000
C	1.99538000	1.54545000	-2.48196000
C	2.14538000	0.14082000	-2.81190000
C	-2.65133000	2.32737000	0.28885000
C	-3.32620000	1.17776000	-0.28344000
C	-3.45442000	0.17139000	0.75338000
C	-2.85904000	0.69901000	1.96634000
C	-2.36292000	2.03167000	1.67936000
C	-0.04679000	2.85801000	-2.08745000
C	-1.46056000	2.64856000	-1.83872000
C	-1.73884000	3.04690000	-0.47201000
C	-0.49706000	3.50210000	0.12390000
C	0.54862000	3.38552000	-0.87457000
C	-2.90974000	-0.60828000	-1.92228000
C	-3.05972000	0.79633000	-1.59228000
C	-2.10652000	1.54771000	-2.38663000
C	-1.36751000	0.60755000	-3.20771000
C	-1.86379000	-0.72502000	-2.92068000
Cl	0.00054000	-0.00021000	-0.00056000

RC-C60: E = -2519.5877474

C	-2.07991000	2.14497000	2.47444000
C	-0.89940000	1.62857000	3.14446000
C	0.26626000	2.25921000	2.54888000
C	-0.19416000	3.16494000	1.51098000
C	-1.64408000	3.09400000	1.46479000
C	0.63536000	2.65334000	-1.92391000
C	-0.15815000	3.37252000	-0.94236000
C	0.53280000	3.30170000	0.33377000
C	1.75369000	2.53917000	0.14046000
C	1.81708000	2.13792000	-1.25415000
C	-1.97262000	-0.58354000	3.26346000
C	-1.44804000	-1.89028000	2.90645000

C	0.00198000	-1.82032000	2.95323000
C	0.37331000	-0.47056000	3.33823000
C	-0.84701000	0.29426000	3.52997000
C	1.65955000	0.09425000	-2.62281000
C	2.31405000	0.88453000	-1.59435000
C	2.76661000	-0.02125000	-0.55678000
C	2.40353000	-1.37144000	-0.94266000
C	1.71503000	-1.30070000	-2.21949000
C	0.53030000	0.58891000	-3.26339000
C	-0.59589000	-0.28940000	-3.52905000
C	-1.81555000	0.47491000	-3.33596000
C	-1.44320000	1.82509000	-2.95063000
C	0.00652000	1.89611000	-2.90577000
C	-3.15786000	1.30499000	2.21977000
C	-3.84836000	1.37644000	0.94393000
C	-4.22020000	0.02621000	0.55857000
C	-3.75961000	-0.87960000	1.59626000
C	-3.10282000	-0.08929000	2.62277000
C	1.43320000	1.52750000	2.36444000
C	1.48827000	0.13254000	2.76751000
C	2.28094000	-0.58726000	1.78714000
C	2.71249000	0.36171000	0.77607000
C	2.19136000	1.66904000	1.13330000
C	-2.30531000	3.16273000	0.24406000
C	-1.54604000	3.30468000	-0.98595000
C	-2.20263000	2.51420000	-2.01219000
C	-3.36786000	1.88383000	-1.41660000
C	-3.43149000	2.28480000	-0.02200000
C	-2.93089000	-0.12801000	-2.76610000
C	-2.87599000	-1.52227000	-2.36305000
C	-3.63523000	-1.66403000	-1.13287000
C	-4.15962000	-0.35736000	-0.77604000
C	-3.72422000	0.59198000	-1.78541000
C	0.10484000	-3.29944000	0.98725000
C	0.86454000	-3.15851000	-0.24279000
C	1.99182000	-2.28156000	0.02362000
C	1.92820000	-1.88039000	1.41966000
C	0.76188000	-2.50887000	2.01394000
C	-3.19413000	-2.53095000	-0.13995000
C	-1.97385000	-3.29498000	-0.33227000
C	-1.28304000	-3.36606000	0.94331000
C	-2.07664000	-2.64641000	1.92413000
C	-3.25763000	-2.12994000	1.25463000
C	0.63785000	-2.14113000	-2.47430000
C	0.20293000	-3.08983000	-1.46395000
C	-1.24703000	-3.15911000	-1.50931000
C	-1.70838000	-2.25359000	-2.54739000
C	-0.54338000	-1.62390000	-3.14364000
C	5.79951000	-0.61641000	1.29124000
C	5.65730000	-1.44502000	0.24658000
C	5.85468000	-0.95658000	-1.12481000
C	5.95927000	0.35714000	-1.38024000

H	5.66610000	-0.98694000	2.31090000
H	5.39385000	-2.49387000	0.39967000
H	5.88959000	-1.68171000	-1.94060000
H	6.06768000	0.70923000	-2.40925000
C	5.85689000	1.38090000	-0.27910000
H	4.81793000	1.76050000	-0.26670000
H	6.48528000	2.25318000	-0.50923000
C	6.23507000	0.81467000	1.09592000
H	7.33377000	0.84758000	1.22007000
H	5.82448000	1.45380000	1.89148000

RC-Li_2F^+@C_{60}: E = -2634.4559854

C	3.25505000	-2.33907000	0.81551000
C	3.26590000	-1.45137000	1.97226000
C	2.08523000	-1.73292000	2.77028000
C	1.33603000	-2.78897000	2.10829000
C	2.05932000	-3.17375000	0.90093000
C	-1.95194000	-2.21247000	0.82606000
C	-0.79358000	-3.08772000	0.90045000
C	-0.05571000	-2.75054000	2.10531000
C	-0.75974000	-1.66647000	2.77273000
C	-1.93124000	-1.33450000	1.98546000
C	4.16852000	0.35038000	0.54925000
C	3.74722000	1.73484000	0.42182000
C	3.03176000	2.10034000	1.62965000
C	3.01050000	0.94215000	2.50434000
C	3.71293000	-0.14058000	1.83745000
C	-2.78942000	0.50067000	0.57833000
C	-2.33834000	-0.00995000	1.86404000
C	-1.59209000	1.04332000	2.53091000
C	-1.58374000	2.21673000	1.66234000
C	-2.32501000	1.87782000	0.44923000
C	-2.78723000	-0.33732000	-0.53214000
C	-2.33621000	0.15048000	-1.82022000
C	-1.63464000	-0.93329000	-2.48867000
C	-1.65459000	-2.09115000	-1.61367000
C	-2.36639000	-1.72223000	-0.40401000
C	3.68599000	-1.85947000	-0.42597000
C	2.94508000	-2.19482000	-1.63607000
C	2.96395000	-1.02980000	-2.51023000
C	3.71341000	0.02153000	-1.84623000
C	4.15664000	-0.48685000	-0.55968000
C	1.41052000	-0.69381000	3.40344000
C	1.88618000	0.67120000	3.27221000
C	0.72937000	1.54767000	3.19701000
C	-0.46347000	0.72207000	3.28134000
C	-0.04120000	-0.66143000	3.40933000
C	1.34695000	-3.49384000	-0.26218000
C	-0.11076000	-3.44840000	-0.25830000
C	-0.55171000	-2.93555000	-1.54487000
C	0.62646000	-2.65273000	-2.34652000

C	1.80203000	-2.99482000	-1.55711000
C	-0.50813000	-0.66007000	-3.25123000
C	-0.03392000	0.70541000	-3.38518000
C	1.41642000	0.67396000	-3.39019000
C	1.83883000	-0.70996000	-3.26032000
C	0.64848000	-1.53597000	-3.17482000
C	1.48582000	3.45134000	0.27514000
C	0.03077000	3.48968000	0.28116000
C	-0.42916000	3.00402000	1.57685000
C	0.74962000	2.66054000	2.36353000
C	1.92753000	2.94181000	1.56039000
C	2.13443000	1.67840000	-2.75668000
C	1.43021000	2.75850000	-2.08824000
C	2.16615000	3.09270000	-0.88264000
C	3.32322000	2.21865000	-0.80767000
C	3.30457000	1.34433000	-1.96594000
C	-1.87846000	2.34344000	-0.79358000
C	-0.67772000	3.16570000	-0.87858000
C	0.04063000	2.79445000	-2.09005000
C	-0.70913000	1.74288000	-2.75234000
C	-1.89091000	1.46067000	-1.95407000
F	0.95248000	0.23668000	-0.33915000
Li	-0.24465000	1.16824000	0.27263000
Li	1.48925000	-1.28475000	-0.07174000
C	-6.40184000	1.11657000	0.55722000
C	-5.91464000	-0.02977000	1.40575000
C	-5.87507000	1.06119000	-0.88114000
H	-5.89344000	0.09353000	2.49170000
H	-6.49353000	1.69442000	-1.53236000
C	-5.62577000	-1.22009000	0.85385000
C	-5.81810000	-0.34312000	-1.42176000
H	-5.35385000	-2.07290000	1.48049000
H	-5.84668000	-0.48887000	-2.50466000
C	-5.69975000	-1.40166000	-0.59979000
H	-5.64219000	-2.41314000	-1.00795000
H	-7.50648000	1.07036000	0.54738000
H	-6.14827000	2.08169000	1.01850000
H	-4.85809000	1.50051000	-0.93411000

RC-LiF_2^-@C_{60}: E = -2726.9994302

C	4.22835600	0.47908100	-0.48786000
C	3.96332200	-0.63918700	-1.38610800
C	3.20237000	-0.12106900	-2.51560400
C	3.00696200	1.30418900	-2.33002100
C	3.63672900	1.67398000	-1.07707500
C	-0.25212200	2.76889100	-1.98724200
C	1.19349600	2.92627700	-1.90086000
C	1.81993600	1.91715100	-2.73286300
C	0.75605900	1.13877500	-3.33582500

C	-0.52245000	1.66037900	-2.87751800
C	3.58745700	-2.08497600	0.58738700
C	2.45779500	-2.96511500	0.86568700
C	1.82789400	-3.32053300	-0.39119400
C	2.55561000	-2.65597000	-1.45378400
C	3.64634400	-1.89156100	-0.86030900
C	-2.44436800	1.01855500	-1.44728800
C	-1.58408700	0.80394400	-2.60430800
C	-1.39223700	-0.62316600	-2.77745400
C	-2.12522200	-1.29919200	-1.72429100
C	-2.78158100	-0.29338000	-0.89901700
C	-2.18776400	2.09101100	-0.59148000
C	-2.24587800	1.89698600	0.85458600
C	-1.15742000	2.66271900	1.45077000
C	-0.42878300	3.33022700	0.38739700
C	-1.05983500	2.97132800	-0.87112900
C	4.17179300	0.29596000	0.89317400
C	3.51816400	1.30459500	1.71829500
C	2.78968100	0.62840500	2.77466900
C	2.98614700	-0.79935700	2.60205500
C	3.84757600	-1.01579500	1.44596600
C	2.17366800	-0.86244400	-3.08339700
C	1.84334000	-2.16113000	-2.54109000
C	0.40021900	-2.31691400	-2.62455100
C	-0.16664000	-1.12138100	-3.21547400
C	0.93406100	-0.22438900	-3.50015100
C	3.03446800	2.64650600	-0.28230400
C	1.79277100	3.28460200	-0.70105300
C	0.95813500	3.48950900	0.46972300
C	1.69298800	2.97842500	1.61426300
C	2.97343500	2.45663600	1.15326400
C	-0.44564700	2.16912300	2.54198000
C	-0.77701600	0.87023100	3.08814500
C	0.46291400	0.23332200	3.50551600
C	1.56525200	1.13003900	3.21888500
C	0.99970200	2.32740200	2.62557900
C	-0.38898700	-3.26380300	0.69440000
C	-1.63037500	-2.62930200	0.27709100
C	-1.56987400	-2.44019500	-1.15435600
C	-0.29009000	-2.95855100	-1.61234800
C	0.44396100	-3.46733200	-0.47201900
C	0.64189100	-1.12811700	3.32521100
C	-0.42026500	-1.90727500	2.72292400
C	0.20718900	-2.91598300	1.89338600
C	1.65062500	-2.76148200	1.97941400
C	1.92004800	-1.65131000	2.86663100
C	-2.83440900	-0.47605400	0.48268700
C	-2.24192400	-1.66786400	1.07262500
C	-1.60809900	-1.29831300	2.32363200
C	-1.79882000	0.12623400	2.50880500
C	-2.55790400	0.64225900	1.37681900
Li	0.93607900	0.86441200	0.16933100

F	1.83603900	-0.44627000	0.02870500
F	-0.49981000	0.21989000	-0.08631900
C	-6.07191900	-1.41085200	-0.41063500
C	-6.26075700	-1.02962700	1.03466300
C	-6.31111800	-0.23894100	-1.37175500
H	-6.45859900	-1.82283500	1.76023600
H	-5.82664500	-0.44609500	-2.33748200
C	-6.09963500	0.23606700	1.44788200
C	-5.83347400	1.08373100	-0.82533800
H	-6.17779500	0.48450400	2.50847700
H	-5.57822200	1.87877500	-1.53018100
C	-5.76636500	1.30385000	0.49453800
H	-5.44455300	2.27310400	0.88044300
H	-5.03790500	-1.78395800	-0.52327800
H	-6.72878700	-2.25242900	-0.67646000
H	-7.39357000	-0.14588900	-1.58530400

RC-Li^{+}@C$_{60}$: E = -2526.9188512

C	1.80569000	1.03041000	-3.22117000
C	0.64040000	0.22358000	-3.54009000
C	-0.54409000	0.97950000	-3.16686000
C	-0.11041000	2.25137000	-2.61696000
C	1.34172000	2.28288000	-2.65021000
C	-0.75045000	3.13539000	0.78440000
C	-0.05858000	3.43653000	-0.45730000
C	-0.79471000	2.81604000	-1.54567000
C	-1.94263000	2.13182000	-0.97791000
C	-1.91595000	2.32923000	0.46450000
C	1.87573000	-1.78845000	-2.83923000
C	1.46993000	-2.86342000	-1.94981000
C	0.01776000	-2.89375000	-1.91620000
C	-0.47336000	-1.83632000	-2.78342000
C	0.67550000	-1.15363000	-3.35543000
C	-1.54792000	1.03008000	2.52745000
C	-2.30645000	1.30057000	1.31724000
C	-2.74753000	0.02715000	0.76642000
C	-2.25205000	-1.03243000	1.63624000
C	-1.51147000	-0.40999000	2.72447000
C	-0.42827000	1.79867000	2.82834000
C	0.77322000	1.16497000	3.34596000
C	1.92102000	1.85047000	2.77772000
C	1.42916000	2.90640000	1.90972000
C	-0.02283000	2.87487000	1.94084000
C	2.95271000	0.42357000	-2.72412000
C	3.69062000	1.04293000	-1.63695000
C	4.18161000	-0.01312000	-0.76896000
C	3.74729000	-1.28534000	-1.31933000
C	2.98800000	-1.01581000	-2.52838000
C	-1.64758000	0.32581000	-2.62729000

C	-1.61108000	-1.11449000	-2.43159000
C	-2.30751000	-1.41841000	-1.19016000
C	-2.77960000	-0.16219000	-0.61795000
C	-2.36314000	0.91518000	-1.50799000
C	2.04556000	2.87348000	-1.60782000
C	1.33035000	3.46139000	-0.48752000
C	2.09033000	3.19204000	0.72130000
C	3.27430000	2.43791000	0.34798000
C	3.24663000	2.24112000	-1.09096000
C	3.05150000	1.12661000	2.41861000
C	3.08682000	-0.31264000	2.61495000
C	3.80152000	-0.90072000	1.49484000
C	4.20815000	0.17507000	0.60743000
C	3.74462000	1.42776000	1.17814000
C	0.11111000	-3.45789000	0.48207000
C	-0.60320000	-2.87087000	1.60409000
C	-1.81027000	-2.23939000	1.08958000
C	-1.83739000	-2.43659000	-0.35761000
C	-0.64776000	-3.18831000	-0.72861000
C	3.38913000	-2.11884000	0.96870000
C	2.23964000	-2.80111000	1.53792000
C	1.50148000	-3.41948000	0.44986000
C	2.19503000	-3.11937000	-0.79148000
C	3.36146000	-2.31549000	-0.47024000
C	-0.35791000	-1.01673000	3.21321000
C	0.10545000	-2.27065000	2.64225000
C	1.55750000	-2.23971000	2.61152000
C	1.99144000	-0.96777000	3.16398000
C	0.80830000	-0.21160000	3.53652000
C	-5.86838000	-0.76592000	-1.18963000
C	-5.64567000	-1.45647000	-0.05774000
C	-5.72765000	-0.79347000	1.24679000
C	-5.78835000	0.54790000	1.33343000
H	-5.84026000	-1.27303000	-2.15777000
H	-5.42112000	-2.52511000	-0.09530000
H	-5.72376000	-1.40560000	2.15117000
H	-5.82406000	1.03403000	2.31182000
Li	-0.59900000	-0.52852000	0.08576000
C	-5.77414000	1.41156000	0.09933000
H	-4.73693000	1.76430000	-0.06767000
H	-6.36049000	2.32532000	0.26871000
C	-6.29329000	0.67851000	-1.14234000
H	-7.39879000	0.69492000	-1.14722000
H	-5.98391000	1.20850000	-2.05443000

RC-Cl$^-$@C_{60}: E = -2979.9494338

C	2.14390000	3.18038000	-0.56517000
C	0.94532000	3.25143000	-1.37894000
C	-0.19226000	3.39386000	-0.48953000
C	0.30354000	3.41027000	0.87403000

C	1.74731000	3.27857000	0.82691000
C	-0.55134000	0.85199000	3.20710000
C	0.27193000	2.00430000	2.89233000
C	-0.41826000	2.78734000	1.88462000
C	-1.66812000	2.11895000	1.57608000
C	-1.75032000	0.92281000	2.39305000
C	1.92403000	1.59415000	-2.90971000
C	1.34548000	0.38119000	-3.45608000
C	-0.09854000	0.51255000	-3.41017000
C	-0.41214000	1.80660000	-2.83504000
C	0.83784000	2.47517000	-2.52566000
C	-1.68285000	-1.52459000	2.13682000
C	-2.30195000	-0.23979000	1.86884000
C	-2.78894000	-0.25695000	0.50464000
C	-2.48279000	-1.55112000	-0.06952000
C	-1.79529000	-2.33511000	0.93866000
C	-0.53511000	-1.59138000	2.91526000
C	0.55166000	-2.47208000	2.53036000
C	1.80116000	-1.80305000	2.83867000
C	1.48678000	-0.50892000	3.41403000
C	0.04307000	-0.37761000	3.46143000
C	3.18448000	2.33694000	-0.93313000
C	3.87432000	1.55406000	0.07453000
C	4.18903000	0.26004000	-0.50068000
C	3.69300000	0.24301000	-1.86392000
C	3.07196000	1.52654000	-2.13069000
C	-1.38899000	2.75430000	-0.78565000
C	-1.50129000	1.94280000	-1.98379000
C	-2.32375000	0.79017000	-1.67004000
C	-2.71466000	0.88736000	-0.27702000
C	-2.14124000	2.10143000	0.26952000
C	2.40843000	2.52930000	1.79177000
C	1.65459000	1.87798000	2.84620000
C	2.27489000	0.59443000	3.11315000
C	3.41235000	0.45250000	2.22406000
C	3.49481000	1.64830000	1.40726000
C	2.89036000	-1.93897000	1.98745000
C	2.77811000	-2.74989000	0.78976000
C	3.53174000	-2.09816000	-0.26471000
C	4.11002000	-0.88510000	0.28162000
C	3.71356000	-0.78665000	1.67356000
C	-0.26624000	-1.87476000	-2.84144000
C	-1.02033000	-2.52670000	-1.78745000
C	-2.10752000	-1.64589000	-1.40357000
C	-2.02560000	-0.44967000	-2.22144000
C	-0.88694000	-0.59101000	-3.10884000
C	3.05623000	-2.11429000	-1.56965000
C	1.80658000	-2.78280000	-1.87854000
C	1.11641000	-2.00020000	-2.88618000
C	1.93981000	-0.84778000	-3.20034000
C	3.13851000	-0.91843000	-2.38659000
C	-0.75499000	-3.17838000	0.57028000

C	-0.35903000	-3.27597000	-0.82216000
C	1.08484000	-3.40662000	-0.86882000
C	1.58128000	-3.39030000	0.49440000
C	0.44417000	-3.24890000	1.38391000
C	-5.74923000	0.23147000	-1.41484000
C	-5.67680000	-1.04813000	-1.02489000
C	-5.97723000	-1.42389000	0.36375000
C	-6.12145000	-0.48961000	1.31508000
H	-5.51632000	0.50720000	-2.44636000
H	-5.37127000	-1.82694000	-1.72637000
H	-6.04157000	-2.48391000	0.61842000
H	-6.29231000	-0.78616000	2.35324000
Cl	0.69526000	0.00375000	0.00270000
C	-5.95713000	0.97657000	1.00996000
H	-4.93115000	1.26925000	1.29843000
H	-6.62635000	1.57572000	1.64554000
C	-6.20667000	1.31315000	-0.46735000
H	-7.28936000	1.47149000	-0.63558000
H	-5.71816000	2.26640000	-0.71853000

TS-C60: E = -2519.5591451

C	-0.12968000	-2.41041000	2.47997000
C	1.32152000	-2.44422000	2.47996000
C	1.80006000	-1.23203000	3.12278000
C	0.64374000	-0.44791000	3.51723000
C	-0.54719000	-1.17862000	3.11480000
C	0.67704000	0.93769000	3.42053000
C	2.94046000	-0.59562000	2.64565000
C	2.00553000	-2.96726000	1.38828000
C	-0.83843000	-2.89453000	1.38341000
C	-1.64916000	-0.48693000	2.62195000
C	-0.47927000	1.66098000	2.91672000
C	-1.61470000	0.95908000	2.51995000
C	-1.99680000	-2.17964000	0.88720000
C	-2.39154000	-0.99499000	1.48809000
C	-0.12300000	-3.44070000	0.24325000
C	1.26686000	-3.47703000	0.24580000
C	3.19631000	-2.30304000	0.89128000
C	3.65387000	-1.14292000	1.50571000
C	1.86790000	1.60320000	2.92370000
C	2.97509000	0.85310000	2.54346000
C	3.70968000	1.20076000	1.34018000
C	4.12979000	-0.03253000	0.69892000
C	-1.99647000	-2.28294000	-0.57137000
C	-0.83807000	-3.06040000	-0.96244000
C	2.00534000	-3.13294000	-0.95709000
C	3.19625000	-2.40580000	-0.55857000
C	-2.33331000	1.33582000	1.32544000
C	-2.93119000	0.13231000	0.71247000
C	-0.00796000	2.76945000	2.11812000

C	1.44320000	2.73403000	2.11547000
C	-1.88952000	2.40189000	0.56673000
C	-0.69804000	3.12253000	0.95919000
C	-2.93120000	0.03045000	-0.72364000
C	-2.39143000	-1.19483000	-1.33283000
C	-0.12987000	-2.73553000	-2.11666000
C	1.32133000	-2.76873000	-2.11168000
C	3.65383000	-1.34361000	-1.33020000
C	4.12961000	-0.13070000	-0.68767000
C	2.14614000	3.06480000	0.96241000
C	3.30265000	2.28265000	0.56700000
C	3.30271000	2.17997000	-0.88259000
C	3.70900000	0.99986000	-1.49597000
C	2.94033000	-0.96203000	-2.53569000
C	1.79970000	-1.65905000	-2.91838000
C	-0.54758000	-1.60497000	-2.91806000
C	-1.64945000	-0.85099000	-2.52697000
C	-2.33344000	1.13585000	-1.49986000
C	-1.88970000	2.29799000	-0.89871000
C	0.03786000	3.46773000	-0.24511000
C	1.42774000	3.44131000	-0.24322000
C	2.97446000	0.48668000	-2.63844000
C	0.64336000	-0.93820000	-3.41943000
C	-1.61477000	0.59496000	-2.62960000
C	-0.69831000	2.95673000	-1.38883000
C	2.14632000	2.89893000	-1.38385000
C	-0.47965000	1.23423000	-3.12148000
C	-0.00819000	2.44402000	-2.48632000
C	0.67661000	0.44727000	-3.51836000
C	1.86738000	1.17614000	-3.12018000
C	1.44292000	2.40917000	-2.47854000
H	-4.94418000	0.32990000	2.43015000
C	-5.10460000	0.22231000	1.35372000
C	-5.42492000	1.23643000	-0.79829000
C	-5.46627000	-1.27048000	-0.68201000
C	-5.10220000	0.02003000	-1.37157000
C	-5.47004000	-1.15526000	0.86167000
C	-5.42536000	1.34089000	0.60664000
H	-6.47451000	-1.54038000	-1.03312000
H	-4.94101000	-0.03236000	-2.45200000
H	-4.81279000	-1.90687000	1.32020000
H	-5.44098000	2.32719000	1.07453000
H	-5.44059000	2.14257000	-1.40705000
H	-4.80469000	-2.07952000	-1.02106000
H	-6.48090000	-1.36701000	1.24387000

TS-Li_2F^+@C_{60}: E = -2634.4349121

C	3.30600000	-2.12484000	0.98793000
C	3.29258000	-1.13049000	2.05318000
C	2.13854000	-1.38692000	2.89397000

C	1.43018000	-2.53366000	2.34758000
C	2.15813000	-3.00510000	1.17300000
C	-1.89324000	-2.24917000	1.06628000
C	-0.69506000	-3.04877000	1.20731000
C	0.03863000	-2.55756000	2.36119000
C	-0.70797000	-1.44780000	2.93292000
C	-1.90224000	-1.25082000	2.14343000
C	4.09531000	0.56062000	0.44877000
C	3.60876000	1.90584000	0.19389000
C	2.89226000	2.35525000	1.37205000
C	2.93605000	1.28805000	2.35539000
C	3.67888000	0.17863000	1.78519000
C	-2.97142000	0.40259000	0.59559000
C	-2.36521000	0.02894000	1.88908000
C	-1.65709000	1.16496000	2.43520000
C	-1.71383000	2.24104000	1.45648000
C	-2.46260000	1.75468000	0.30540000
C	-2.95899000	-0.57768000	-0.46301000
C	-2.42053000	-0.17794000	-1.77045000
C	-1.66650000	-1.27796000	-2.33837000
C	-1.62059000	-2.34285000	-1.35777000
C	-2.34293000	-1.89388000	-0.19050000
C	3.70407000	-1.75287000	-0.29875000
C	2.97097000	-2.24470000	-1.45727000
C	2.92297000	-1.17007000	-2.44011000
C	3.62714000	-0.02388000	-1.89352000
C	4.10922000	-0.38172000	-0.57175000
C	1.42469000	-0.32362000	3.43642000
C	1.83607000	1.04254000	3.16563000
C	0.63871000	1.85163000	3.02279000
C	-0.51045000	0.98005000	3.20642000
C	-0.02537000	-0.35645000	3.46547000
C	1.45450000	-3.48546000	0.06056000
C	-0.00378000	-3.50562000	0.08187000
C	-0.48072000	-3.13700000	-1.23345000
C	0.67203000	-2.88146000	-2.08300000
C	1.87315000	-3.09460000	-1.28549000
C	-0.56858000	-1.03622000	-3.15532000
C	-0.16502000	0.32484000	-3.43336000
C	1.28416000	0.36283000	-3.45712000
C	1.77617000	-0.98082000	-3.20207000
C	0.62890000	-1.84999000	-3.01547000
C	1.26578000	3.49368000	-0.08155000
C	-0.18989000	3.46346000	-0.05552000
C	-0.60555000	3.07881000	1.28281000
C	0.59609000	2.87545000	2.08514000
C	1.74842000	3.13419000	1.24021000
C	1.95905000	1.45672000	-2.93239000
C	1.21093000	2.56208000	-2.35987000
C	1.94891000	3.05372000	-1.20952000
C	3.14774000	2.24791000	-1.06978000
C	3.15384000	1.26012000	-2.13448000

C	-2.06356000	2.13052000	-0.97961000
C	-0.90344000	2.99151000	-1.16369000
C	-0.17956000	2.53064000	-2.34166000
C	-0.88470000	1.38337000	-2.88448000
C	-2.04409000	1.12783000	-2.05069000
F	1.02758000	0.28861000	-0.09689000
Li	-0.35003000	1.15787000	0.06750000
Li	1.38317000	-1.30601000	-0.02387000
C	-5.54243000	1.37015000	-0.26561000
C	-5.19067000	0.80244000	1.08365000
C	-5.51661000	0.31894000	-1.40088000
H	-5.05570000	1.51977000	1.89845000
H	-6.52104000	0.22721000	-1.84239000
C	-5.46067000	-0.51696000	1.39046000
C	-5.13839000	-1.06065000	-0.92977000
H	-5.48274000	-0.84587000	2.43124000
H	-4.97489000	-1.81519000	-1.70468000
C	-5.43573000	-1.47449000	0.35556000
H	-5.44096000	-2.53797000	0.60278000
H	-6.55839000	1.78351000	-0.16802000
H	-4.89998000	2.23124000	-0.49685000
H	-4.86237000	0.63197000	-2.22645000

TS-LiF_2^-@C_{60}: E = -2726.9712615

C	4.18122000	-0.12776000	-0.68645000
C	3.70542000	-1.37970000	-1.27185000
C	2.95270000	-1.05461000	-2.47499000
C	2.95827000	0.38535000	-2.64121000
C	3.70952000	0.95857000	-1.53797000
C	-0.06664000	2.30628000	-2.58167000
C	1.38887000	2.28605000	-2.57423000
C	1.83446000	1.03387000	-3.15278000
C	0.64631000	0.28438000	-3.51486000
C	-0.52674000	1.06727000	-3.15848000
C	3.24310000	-2.23126000	0.99843000
C	2.03606000	-2.85901000	1.51555000
C	1.29381000	-3.41899000	0.40557000
C	2.03924000	-3.13567000	-0.80371000
C	3.24668000	-2.40506000	-0.44774000
C	-2.41266000	1.04109000	-1.55145000
C	-1.66582000	0.45002000	-2.64195000
C	-1.68051000	-0.98746000	-2.47029000
C	-2.43888000	-1.28740000	-1.27316000
C	-2.99858000	-0.03798000	-0.72051000
C	-1.98272000	2.24073000	-1.00762000
C	-1.98402000	2.41394000	0.45308000
C	-0.77944000	3.14463000	0.80750000
C	-0.03548000	3.43117000	-0.40749000
C	-0.77747000	2.86753000	-1.52153000
C	4.17992000	0.03710000	0.70056000

C	3.70674000	1.29179000	1.27379000
C	2.95383000	0.99327000	2.48038000
C	2.94656000	-0.44559000	2.65392000
C	3.69976000	-1.04176000	1.56017000
C	1.80500000	-1.76518000	-2.81557000
C	1.33696000	-2.83431000	-1.96156000
C	-0.11666000	-2.81498000	-1.96603000
C	-0.55510000	-1.73430000	-2.81539000
C	0.63338000	-1.08794000	-3.34356000
C	3.27656000	2.16230000	-0.98626000
C	2.09816000	2.83508000	-1.51401000
C	1.36298000	3.41911000	-0.40566000
C	2.09575000	3.11028000	0.81036000
C	3.27491000	2.33281000	0.45492000
C	-0.07096000	2.84831000	1.97249000
C	-0.53245000	1.77797000	2.82337000
C	0.64064000	1.09987000	3.35454000
C	1.82987000	1.74414000	2.82763000
C	1.38557000	2.82718000	1.97122000
C	-0.83204000	-2.81673000	1.50852000
C	-2.01682000	-2.15607000	0.98950000
C	-2.01585000	-2.32852000	-0.46013000
C	-0.83038000	-3.09150000	-0.80888000
C	-0.09971000	-3.39821000	0.40285000
C	0.62747000	-0.27552000	3.50746000
C	-0.56050000	-1.02826000	3.14391000
C	-0.12073000	-2.27770000	2.57088000
C	1.33273000	-2.29711000	2.57162000
C	1.79933000	-1.05725000	3.15207000
C	-3.00014000	0.13131000	0.70643000
C	-2.44197000	-0.95416000	1.53661000
C	-1.68534000	-0.38249000	2.63193000
C	-1.67112000	1.05583000	2.46309000
C	-2.41634000	1.37545000	1.26312000
Li	0.72576000	0.88376000	0.05768000
F	1.79858000	-0.29551000	-0.00701000
F	-0.63383000	0.04261000	-0.00762000
C	-5.55083000	-1.16499000	0.91398000
C	-5.22986000	0.24444000	1.34646000
C	-5.54734000	-1.34912000	-0.62362000
H	-5.06304000	0.40127000	2.41560000
H	-4.85543000	-2.14824000	-0.92360000
C	-5.56203000	1.31777000	0.54930000
C	-5.22317000	-0.08156000	-1.37510000
H	-5.57092000	2.32636000	0.96788000
H	-5.05182000	-0.18149000	-2.45032000
C	-5.55876000	1.14946000	-0.85551000
H	-5.56502000	2.03062000	-1.50052000
H	-4.86052000	-1.87017000	1.39727000
H	-6.55344000	-1.40010000	1.30748000
H	-6.54832000	-1.67082000	-0.95502000

TS-Li^+@C_{60}: E = -2526.8978789

C	-0.13243000	-2.22764000	-2.64558000
C	1.31930000	-2.22518000	-2.68728000
C	1.80337000	-2.98588000	-1.54795000
C	0.65064000	-3.45524000	-0.79966000
C	-0.54425000	-2.98103000	-1.48061000
C	0.69127000	-3.49918000	0.58852000
C	2.94494000	-2.57236000	-0.87119000
C	1.99935000	-1.08488000	-3.09890000
C	-0.84305000	-1.08806000	-3.01499000
C	-1.64828000	-2.56620000	-0.73955000
C	-0.46196000	-3.06766000	1.36284000
C	-1.60623000	-2.61074000	0.71015000
C	-1.99687000	-0.66620000	-2.24554000
C	-2.39615000	-1.38659000	-1.12799000
C	-0.13148000	0.10185000	-3.44928000
C	1.25776000	0.10307000	-3.48787000
C	3.19432000	-0.65619000	-2.39548000
C	3.65681000	-1.38336000	-1.30504000
C	1.88527000	-3.07212000	1.29612000
C	2.98622000	-2.61557000	0.58095000
C	3.72323000	-1.45250000	1.04319000
C	4.13829000	-0.69146000	-0.12194000
C	-1.99712000	0.79759000	-2.20215000
C	-0.84339000	1.26397000	-2.94540000
C	1.99935000	1.26612000	-3.02954000
C	3.19437000	0.79678000	-2.35245000
C	-2.33218000	-1.46038000	1.21085000
C	-2.94509000	-0.72928000	0.07609000
C	0.01580000	-2.38324000	2.54459000
C	1.46768000	-2.37986000	2.50398000
C	-1.87190000	-0.80615000	2.34598000
C	-0.67312000	-1.26750000	3.01995000
C	-2.94478000	0.72330000	0.11921000
C	-2.39650000	1.45093000	-1.04398000
C	-0.13262000	2.37976000	-2.50969000
C	1.31918000	2.37991000	-2.55137000
C	3.65679000	1.45819000	-1.22099000
C	4.13826000	0.69755000	-0.08082000
C	2.17129000	-1.26390000	2.94275000
C	3.32514000	-0.79194000	2.19990000
C	3.32503000	0.66075000	2.24300000
C	3.72324000	1.38834000	1.12732000
C	2.94480000	2.61948000	-0.71773000
C	1.80324000	3.07205000	-1.36894000
C	-0.54429000	3.06322000	-1.30231000
C	-1.64843000	2.60565000	-0.58684000
C	-2.33217000	1.38630000	1.29500000
C	-1.87188000	0.66634000	2.38976000

C	0.06429000	-0.10279000	3.48106000
C	1.45422000	-0.10155000	3.44104000
C	2.98629000	2.57663000	0.73440000
C	0.65049000	3.49640000	-0.59446000
C	-1.60641000	2.56425000	0.86294000
C	-0.67315000	1.08708000	3.08964000
C	2.17107000	1.08822000	3.01238000
C	-0.46206000	2.98177000	1.54144000
C	0.01572000	2.22901000	2.68068000
C	0.69117000	3.45830000	0.79387000
C	1.88528000	2.99036000	1.47501000
C	1.46752000	2.22808000	2.63983000
H	-4.97287000	-2.45687000	0.06502000
C	-5.12445000	-1.37348000	0.07026000
C	-5.42921000	0.66285000	1.30942000
C	-5.47966000	0.81162000	-1.19737000
C	-5.12760000	1.36601000	0.15718000
C	-5.47677000	-0.73490000	-1.24680000
C	-5.42820000	-0.74520000	1.26466000
H	-6.48821000	1.18803000	-1.42853000
H	-4.97691000	2.44766000	0.22061000
H	-4.81844000	-1.11322000	-2.04113000
H	-5.45672000	-1.31655000	2.19468000
H	-5.45815000	1.17377000	2.27394000
H	-4.82404000	1.24238000	-1.96681000
H	-6.48353000	-1.09941000	-1.50331000
Li	-0.74569000	-0.00899000	0.36002000

TS-Cl^-@C_{60}: E = -2979.9161235

C	-0.14913000	-2.57737000	2.30287000
C	1.30050000	-2.60669000	2.30046000
C	1.77453000	-1.44268000	3.02601000
C	0.61767000	-0.69238000	3.47424000
C	-0.56965000	-1.39569000	3.02249000
C	0.64677000	0.69598000	3.47443000
C	2.91213000	-0.77141000	2.59490000
C	1.98531000	-3.04938000	1.17543000
C	-0.85549000	-2.98641000	1.17600000
C	-1.67321000	-0.67510000	2.58075000
C	-0.51023000	1.44860000	3.02376000
C	-1.64307000	0.77349000	2.58047000
C	-2.01492000	-2.24299000	0.73177000
C	-2.40939000	-1.10546000	1.41429000
C	-0.13987000	-3.44821000	0.00174000
C	1.24903000	-3.47987000	0.00171000
C	3.17295000	-2.34974000	0.72698000
C	3.62612000	-1.23476000	1.42082000
C	1.83382000	1.39734000	3.02578000
C	2.94223000	0.67922000	2.59427000
C	3.67475000	1.11185000	1.41976000

C	4.09745000	-0.07058000	0.69448000
C	-2.01498000	-2.24370000	-0.72939000
C	-0.85559000	-2.98757000	-1.17295000
C	1.98525000	-3.05054000	-1.17247000
C	3.17291000	-2.35045000	-0.72480000
C	-2.35800000	1.23080000	1.41511000
C	-2.94951000	0.07160000	0.71883000
C	-0.04330000	2.61043000	2.30429000
C	1.40631000	2.57865000	2.29873000
C	-1.92263000	2.34819000	0.73284000
C	-0.73373000	3.04175000	1.17390000
C	-2.94959000	0.07092000	-0.71871000
C	-2.40953000	-1.10686000	-1.41304000
C	-0.14928000	-2.57966000	-2.30025000
C	1.30036000	-2.60897000	-2.29790000
C	3.62604000	-1.23617000	-1.41977000
C	4.09741000	-0.07127000	-0.69461000
C	2.10785000	2.99158000	1.17291000
C	3.26515000	2.24326000	0.72453000
C	3.26511000	2.24256000	-0.72692000
C	3.67467000	1.11045000	-1.42104000
C	2.91197000	-0.77399000	-2.59427000
C	1.77435000	-1.44570000	-3.02464000
C	-0.56984000	-1.39871000	-3.02103000
C	-1.67337000	-0.67767000	-2.57996000
C	-2.35802000	1.22939000	-1.41615000
C	-1.92266000	2.34748000	-0.73504000
C	0.00005000	3.47166000	-0.00171000
C	1.38892000	3.44908000	-0.00175000
C	2.94208000	0.67664000	-2.59506000
C	0.61746000	-0.69584000	-3.47352000
C	-1.64321000	0.77091000	-2.58111000
C	-0.73379000	3.04058000	-1.17685000
C	2.10778000	2.99042000	-1.17599000
C	-0.51039000	1.44559000	-3.02513000
C	-0.04343000	2.60814000	-2.30687000
C	0.64657000	0.69252000	-3.47515000
C	1.83366000	1.39432000	-3.02724000
C	1.40617000	2.57634000	-2.30136000
H	-4.93637000	0.14894000	2.44211000
C	-5.10773000	0.12189000	1.36248000
C	-5.45208000	1.28931000	-0.70429000
C	-5.47758000	-1.21775000	-0.77406000
C	-5.10769000	0.12181000	-1.36244000
C	-5.47712000	-1.21783000	0.77413000
C	-5.45219000	1.28932000	0.70424000
H	-6.48796000	-1.46152000	-1.14038000
H	-4.93624000	0.14877000	-2.44206000
H	-4.81063000	-1.99671000	1.16953000
H	-5.45944000	2.23925000	1.24259000
H	-5.45917000	2.23924000	-1.24266000
H	-4.81183000	-1.99701000	-1.16990000

H	-6.48710000	-1.46235000	1.14102000
Cl	0.61705000	-0.00486000	0.00001000

CA-C_{60}: E = -2519.6256830

C	-1.43387000	-1.80553000	3.03300000
C	-0.69464000	-0.63979000	3.48163000
C	-1.41168000	0.54120000	3.02767000
C	-2.58458000	0.11056000	2.31017000
C	-2.60283000	-1.34042000	2.30593000
C	-2.98497000	0.81613000	-1.17614000
C	-3.43804000	0.09626000	0.00000000
C	-2.98497000	0.81613000	1.17614000
C	-2.25344000	1.98266000	0.74086000
C	-2.25344000	1.98266000	-0.74086000
C	1.40953000	-1.83463000	3.03321000
C	2.58753000	-1.39277000	2.30605000
C	2.59916000	0.05826000	2.31085000
C	1.43520000	0.51200000	3.02808000
C	0.69398000	-0.65401000	3.48161000
C	-0.70254000	1.65277000	-2.57407000
C	-1.13958000	2.40122000	-1.42688000
C	0.03803000	3.15021000	-0.79890000
C	1.19947000	2.37395000	-1.42528000
C	0.74829000	1.63710000	-2.57328000
C	-1.41168000	0.54120000	-3.02767000
C	-0.69464000	-0.63979000	-3.48163000
C	-1.43387000	-1.80553000	-3.03300000
C	-2.60283000	-1.34042000	-2.30593000
C	-2.58458000	0.11056000	-2.31017000
C	-0.75006000	-2.93673000	2.59975000
C	-1.20543000	-3.65348000	1.42278000
C	-0.03536000	-4.11246000	0.69514000
C	1.14361000	-3.67740000	1.42277000
C	0.70281000	-2.95154000	2.59970000
C	-0.70254000	1.65277000	2.57407000
C	0.74829000	1.63710000	2.57328000
C	1.19947000	2.37395000	1.42528000
C	0.03803000	3.15021000	0.79890000
C	-1.13958000	2.40122000	1.42688000
C	-3.03556000	-2.02772000	1.17671000
C	-3.46877000	-1.29279000	0.00000000
C	-3.03556000	-2.02772000	-1.17671000
C	-2.32465000	-3.20797000	-0.72736000
C	-2.32465000	-3.20797000	0.72736000
C	-0.75006000	-2.93673000	-2.59975000
C	0.70281000	-2.95154000	-2.59970000
C	1.14361000	-3.67740000	-1.42277000
C	-0.03536000	-4.11246000	-0.69514000
C	-1.20543000	-3.65348000	-1.42278000
C	3.45103000	0.02700000	0.00000000

C	3.01269000	0.75607000	-1.17631000
C	2.30559000	1.93724000	-0.74078000
C	2.30559000	1.93724000	0.74078000
C	3.01269000	0.75607000	1.17631000
C	2.27148000	-3.25395000	-0.72733000
C	3.00632000	-2.08853000	-1.17679000
C	3.45418000	-1.36238000	0.00000000
C	3.00632000	-2.08853000	1.17679000
C	2.27148000	-3.25395000	0.72733000
C	1.43520000	0.51200000	-3.02808000
C	2.59916000	0.05826000	-2.31085000
C	2.58753000	-1.39277000	-2.30605000
C	1.40953000	-1.83463000	-3.03321000
C	0.69398000	-0.65401000	-3.48161000
C	0.07830000	4.64584000	1.28246000
C	1.28942000	5.29646000	0.66828000
C	1.28942000	5.29646000	-0.66828000
C	0.07830000	4.64584000	-1.28246000
H	0.11272000	4.64828000	2.38015000
H	2.09107000	5.71554000	1.27794000
H	2.09107000	5.71554000	-1.27794000
H	0.11272000	4.64828000	-2.38015000
C	-1.18470000	5.36724000	-0.77212000
H	-2.07891000	4.86741000	-1.17058000
H	-1.18523000	6.39243000	-1.16532000
C	-1.18470000	5.36724000	0.77212000
H	-1.18523000	6.39243000	1.16532000
H	-2.07891000	4.86741000	1.17058000

CA-Li_2F^+@C_{60}: E = -2634.4992721

C	-3.24379000	1.77433000	1.59029000
C	-3.23285000	0.51574000	2.32624000
C	-2.06720000	0.50866000	3.18589000
C	-1.34918000	1.75653000	2.97902000
C	-2.08449000	2.55299000	2.00129000
C	1.95164000	1.82431000	1.61064000
C	0.76644000	2.55451000	1.99687000
C	0.04159000	1.75873000	2.97090000
C	0.77829000	0.52509000	3.18806000
C	1.95899000	0.54673000	2.35946000
C	-4.07797000	-0.63406000	0.31733000
C	-3.61271000	-1.85415000	-0.31898000
C	-2.89254000	-2.63202000	0.67002000
C	-2.91064000	-1.89140000	1.91852000
C	-3.64232000	-0.65732000	1.70128000
C	3.19588000	-0.65157000	0.44461000
C	2.40988000	-0.60325000	1.75777000
C	1.68265000	-1.82778000	1.95701000
C	1.71465000	-2.58150000	0.70963000
C	2.46370000	-1.80686000	-0.25416000

C	3.18062000	0.72849000	-0.36860000
C	2.42809000	0.66379000	-1.69777000
C	1.67077000	1.87035000	-1.90579000
C	1.64911000	2.60871000	-0.65863000
C	2.39112000	1.85192000	0.31135000
C	-3.66532000	1.79425000	0.25889000
C	-2.94370000	2.59508000	-0.71974000
C	-2.91970000	1.84652000	-1.97005000
C	-3.62898000	0.59659000	-1.76428000
C	-4.09051000	0.56218000	-0.38911000
C	-1.36350000	-0.67316000	3.39231000
C	-1.79758000	-1.90012000	2.74883000
C	-0.61350000	-2.64504000	2.36169000
C	0.54892000	-1.87128000	2.76907000
C	0.08614000	-0.66437000	3.40470000
C	-1.39202000	3.33482000	1.06640000
C	0.06642000	3.33103000	1.06818000
C	0.52155000	3.35185000	-0.30022000
C	-0.64409000	3.36472000	-1.17136000
C	-1.83372000	3.35405000	-0.32853000
C	0.56013000	1.89318000	-2.74636000
C	0.13859000	0.67811000	-3.39447000
C	-1.31066000	0.65793000	-3.40905000
C	-1.78466000	1.87595000	-2.77281000
C	-0.62466000	2.64458000	-2.36140000
C	-1.29526000	-3.32049000	-1.07106000
C	0.16086000	-3.31249000	-1.05559000
C	0.59428000	-3.33405000	0.32576000
C	-0.59563000	-3.35943000	1.17139000
C	-1.76030000	-3.35306000	0.30446000
C	-1.99096000	-0.53592000	-3.20719000
C	-1.24895000	-1.76511000	-2.98312000
C	-1.98202000	-2.56305000	-2.01427000
C	-3.16733000	-1.82155000	-1.63413000
C	-3.17224000	-0.56824000	-2.37019000
C	2.03766000	-1.77938000	-1.56914000
C	0.86952000	-2.53572000	-1.98345000
C	0.14074000	-1.74692000	-2.96728000
C	0.85311000	-0.49781000	-3.16826000
C	2.02222000	-0.49429000	-2.31793000
C	5.42022000	-1.22541000	-0.61827000
C	4.69672000	-1.03104000	0.72868000
C	5.40438000	0.10307000	-1.40557000
H	4.70874000	-1.95740000	1.31830000
H	6.42494000	0.45349000	-1.60463000
C	5.32837000	0.12395000	1.45989000
C	4.67418000	1.17997000	-0.57938000
H	5.75653000	0.00871000	2.45633000
H	4.66807000	2.14217000	-1.10838000
C	5.31761000	1.27396000	0.77893000
H	5.73622000	2.20866000	1.15408000
H	6.44874000	-1.54850000	-0.41399000

H	4.94008000	-2.03503000	-1.18657000
H	4.91169000	-0.01414000	-2.38133000
F	-1.03279000	-0.26805000	-0.05224000
Li	0.30581000	-1.18028000	-0.28116000
Li	-1.31120000	1.30213000	0.30822000

CA-LiF_2^-@C_{60}: E = -2727.0485538

C	4.15416000	-0.66235000	-0.21013000
C	3.69143000	-1.73460000	0.66516000
C	2.94239000	-2.68284000	-0.14408000
C	2.93772000	-2.20750000	-1.51384000
C	3.67941000	-0.96043000	-1.55563000
C	-0.10179000	-1.33127000	-3.19307000
C	1.35262000	-1.32724000	-3.18443000
C	1.80962000	-2.39196000	-2.31263000
C	0.62991000	-3.04877000	-1.78397000
C	-0.54734000	-2.38712000	-2.32540000
C	3.23337000	-0.06094000	2.42013000
C	2.03719000	0.12994000	3.22145000
C	1.29825000	-1.11613000	3.24640000
C	2.04214000	-2.08309000	2.46340000
C	3.23815000	-1.43889000	1.94889000
C	-2.42986000	-0.95946000	-1.59226000
C	-1.67876000	-2.18563000	-1.53182000
C	-1.68273000	-2.65704000	-0.16098000
C	-2.43827000	-1.72695000	0.63316000
C	-3.20059000	-0.75240000	-0.27855000
C	-2.02188000	0.04949000	-2.43716000
C	-2.02390000	1.45554000	-1.95349000
C	-0.82271000	2.08632000	-2.46175000
C	-0.08239000	1.11735000	-3.25182000
C	-0.81962000	-0.13328000	-3.22376000
C	4.15183000	0.65747000	0.24316000
C	3.67483000	1.71907000	-0.63371000
C	2.93041000	2.67620000	0.16542000
C	2.93308000	2.20701000	1.53681000
C	3.68302000	0.96232000	1.58988000
C	1.80330000	-3.30639000	0.35817000
C	1.34090000	-3.00162000	1.69529000
C	-0.11202000	-3.00526000	1.68551000
C	-0.55324000	-3.30035000	0.35098000
C	0.62795000	-3.49190000	-0.47335000
C	3.23676000	0.05830000	-2.39608000
C	2.05548000	-0.12963000	-3.22116000
C	1.31490000	1.11991000	-3.25612000
C	2.05175000	2.08610000	-2.45868000
C	3.23422000	1.43176000	-1.92336000
C	-0.10859000	3.01600000	-1.69981000
C	-0.55682000	3.31507000	-0.36582000
C	0.62062000	3.50592000	0.46924000

C	1.80209000	3.31461000	-0.35132000
C	1.34717000	3.01031000	-1.69503000
C	-0.82926000	0.13648000	3.19372000
C	-2.02167000	-0.04226000	2.39484000
C	-2.02032000	-1.44479000	1.91392000
C	-0.82637000	-2.07428000	2.43391000
C	-0.09404000	-1.11098000	3.22911000
C	0.61816000	3.04687000	1.77548000
C	-0.56231000	2.38670000	2.30755000
C	-0.11883000	1.33310000	3.17807000
C	1.33409000	1.32601000	3.18408000
C	1.79401000	2.38950000	2.31686000
C	-3.20381000	0.75842000	0.24090000
C	-2.44334000	0.96797000	1.55976000
C	-1.69142000	2.19253000	1.50709000
C	-1.68807000	2.66488000	0.13569000
C	-2.43593000	1.73298000	-0.66760000
Li	0.59544000	0.46137000	-0.71761000
F	1.73013000	-0.13741000	0.23268000
F	-0.78529000	0.00596000	-0.01431000
C	-5.40945000	0.32587000	1.40448000
C	-4.69688000	1.22207000	0.37063000
C	-5.40678000	-1.13457000	0.90222000
H	-4.70775000	2.27145000	0.69590000
H	-4.89049000	-1.79502000	1.61301000
C	-5.36330000	1.03120000	-0.96724000
C	-4.69173000	-1.20324000	-0.46319000
H	-5.78616000	1.86680000	-1.52769000
H	-4.69820000	-2.23073000	-0.85206000
C	-5.36075000	-0.23277000	-1.40175000
H	-5.78100000	-0.54885000	-2.35811000
H	-4.89439000	0.41148000	2.37164000
H	-6.43640000	0.69194000	1.54448000
H	-6.43242000	-1.51249000	0.78606000

CA-Li$^+$@C$_{60}$: E = -2526.9609280

C	1.81191000	3.03297000	1.43989000
C	0.64348000	3.47990000	0.70312000
C	-0.53637000	3.02725000	1.42566000
C	-0.10176000	2.31154000	2.59760000
C	1.34961000	2.30688000	2.61077000
C	-0.80608000	-1.17583000	2.99844000
C	-0.08515000	0.00054000	3.45022000
C	-0.80608000	1.17677000	2.99807000
C	-1.97468000	0.74124000	2.26965000
C	-1.97468000	-0.74053000	2.26988000
C	1.83413000	3.03850000	-1.40418000
C	1.38937000	2.30769000	-2.58006000
C	-0.06331000	2.31064000	-2.58785000
C	-0.51278000	3.02807000	-1.42083000

C	0.65582000	3.48735000	-0.68540000
C	-1.65300000	-2.57576000	0.72392000
C	-2.40220000	-1.42786000	1.15965000
C	-3.15497000	-0.80008000	-0.01730000
C	-2.37567000	-1.42382000	-1.17731000
C	-1.63685000	-2.57276000	-0.72822000
C	-0.53637000	-3.02680000	1.42660000
C	0.64348000	-3.47967000	0.70421000
C	1.81191000	-3.03252000	1.44083000
C	1.34962000	-2.30606000	2.61149000
C	-0.10176000	-2.31072000	2.59832000
C	2.94117000	2.60025000	0.75294000
C	3.66018000	1.42359000	1.20614000
C	4.11495000	0.69513000	0.03476000
C	3.67582000	1.42193000	-1.14346000
C	2.95093000	2.59990000	-0.70037000
C	-1.65300000	2.57599000	0.72311000
C	-1.63685000	2.57254000	-0.72902000
C	-2.37567000	1.42345000	-1.17776000
C	-3.15497000	0.80007000	-0.01755000
C	-2.40221000	1.42823000	1.15921000
C	2.03752000	1.17731000	3.03958000
C	1.30356000	0.00055000	3.47495000
C	2.03752000	-1.17636000	3.03995000
C	3.21601000	-0.72720000	2.32520000
C	3.21601000	0.72793000	2.32497000
C	2.94117000	-2.60002000	0.75375000
C	2.95093000	-2.60012000	-0.69955000
C	3.67582000	-1.42228000	-1.14301000
C	4.11495000	-0.69511000	0.03497000
C	3.66018000	-1.42321000	1.20658000
C	-0.04060000	-0.00054000	-3.46032000
C	-0.77111000	-1.18129000	-3.01595000
C	-1.95339000	-0.74383000	-2.30041000
C	-1.95339000	0.74310000	-2.30064000
C	-0.77110000	1.18034000	-3.01631000
C	3.25514000	-0.72782000	-2.27272000
C	2.08512000	-1.17830000	-3.00080000
C	1.35460000	-0.00054000	-3.44602000
C	2.08512000	1.17736000	-3.00117000
C	3.25513000	0.72711000	-2.27295000
C	-0.51277000	-3.02851000	-1.41988000
C	-0.06331000	-2.31145000	-2.58713000
C	1.38937000	-2.30849000	-2.57934000
C	1.83413000	-3.03893000	-1.40323000
C	0.65582000	-3.48756000	-0.68431000
C	-4.65233000	1.28469000	-0.06781000
C	-5.29356000	0.66824000	-1.28286000
C	-5.29355000	-0.66866000	-1.28265000
C	-4.65233000	-1.28471000	-0.06739000
H	-4.65494000	2.38225000	-0.10161000
H	-5.72241000	1.27763000	-2.07946000

H	-5.72241000	-1.27832000	-2.07904000
H	-4.65494000	-2.38228000	-0.10083000
Li	-0.05873000	-0.00034000	-1.16964000
C	-5.37467000	-0.77178000	1.19401000
H	-4.88324000	-1.17323000	2.09153000
H	-6.39910000	-1.16486000	1.18842000
C	-5.37467000	0.77217000	1.19376000
H	-6.39910000	1.16525000	1.18803000
H	-4.88325000	1.17393000	2.09114000

CA-Cl$^-$@C_{60}: E = -2979.9826204

C	1.77651000	-3.02929000	-1.43391000
C	0.61273000	-3.47806000	-0.69543000
C	-0.56690000	-3.02469000	-1.41133000
C	-0.13771000	-2.30701000	-2.58294000
C	1.31156000	-2.30229000	-2.60074000
C	-0.84276000	1.17595000	-2.98255000
C	-0.12366000	0.00134000	-3.43511000
C	-0.84274000	-1.17360000	-2.98343000
C	-2.00964000	-0.73933000	-2.25536000
C	-2.00967000	0.74116000	-2.25481000
C	1.80642000	-3.03052000	1.40682000
C	1.36537000	-2.30424000	2.58341000
C	-0.08394000	-2.30980000	2.59673000
C	-0.53701000	-3.02642000	1.43380000
C	0.62729000	-3.47849000	0.69248000
C	-1.67675000	2.57271000	-0.69959000
C	-2.41914000	1.42488000	-1.13752000
C	-3.16479000	0.79644000	0.03944000
C	-2.39185000	1.42255000	1.20111000
C	-1.66101000	2.57153000	0.74963000
C	-0.56686000	3.02582000	-1.40900000
C	0.61278000	3.47863000	-0.69277000
C	1.77655000	3.03039000	-1.43157000
C	1.31159000	2.30427000	-2.59895000
C	-0.13768000	2.30900000	-2.58116000
C	2.90695000	-2.59625000	-0.75072000
C	3.62296000	-1.42084000	-1.20553000
C	4.08112000	-0.69463000	-0.03650000
C	3.64778000	-1.42182000	1.14110000
C	2.92220000	-2.59677000	0.70037000
C	-1.67679000	-2.57212000	-0.70161000
C	-1.66104000	-2.57210000	0.74762000
C	-2.39183000	-1.42343000	1.19998000
C	-3.16479000	-0.79641000	0.03881000
C	-2.41917000	-1.42393000	-1.13866000
C	1.99837000	-1.17387000	-3.03317000
C	1.26442000	0.00134000	-3.46581000
C	1.99841000	1.17620000	-3.03226000
C	3.17802000	0.72736000	-2.32329000

C	3.17800000	-0.72559000	-2.32386000
C	2.90699000	2.59682000	-0.74872000
C	2.92223000	2.59616000	0.70238000
C	3.64780000	1.42088000	1.14222000
C	4.08113000	0.69461000	-0.03595000
C	3.62299000	1.42174000	-1.20441000
C	-0.05234000	-0.00133000	3.44875000
C	-0.78088000	1.17376000	3.01224000
C	-1.96289000	0.73922000	2.30947000
C	-1.96295000	-0.74100000	2.30893000
C	-0.78092000	-1.17607000	3.01134000
C	3.22527000	0.72553000	2.26931000
C	2.06101000	1.17394000	3.00340000
C	1.33608000	-0.00134000	3.45109000
C	2.06101000	-1.17627000	3.00249000
C	3.22526000	-0.72733000	2.26872000
C	-0.53698000	3.02535000	1.43614000
C	-0.08390000	2.30781000	2.59849000
C	1.36539000	2.30224000	2.58517000
C	1.80646000	3.02940000	1.40914000
C	0.62733000	3.47793000	0.69514000
C	-4.65957000	-1.28078000	0.07787000
C	-5.31529000	-0.66893000	1.28712000
C	-5.31529000	0.66776000	1.28771000
C	-4.65964000	1.28070000	0.07899000
H	-4.66066000	-2.37872000	0.11146000
H	-5.72371000	-1.27885000	2.09459000
H	-5.72373000	1.27694000	2.09573000
H	-4.66080000	2.37861000	0.11355000
Cl	0.59852000	-0.00001000	-0.00308000
C	-5.38246000	0.77272000	-1.18446000
H	-4.87413000	1.16830000	-2.07501000
H	-6.40853000	1.16670000	-1.18909000
C	-5.38250000	-0.77171000	-1.18510000
H	-6.40858000	-1.16563000	-1.18979000
H	-4.87438000	-1.16655000	-2.07610000