Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The effect of intermolecular interaction of the charge transfer complex between molecular tweezer and C_{60}/C_{70} on its second-order nonlinear optical properties

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The detailed description of the Localized orbital locator (LOL) maps.

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†*Electronic supplementary information (ESI) available: The components of the total polarizability α and γ (a.u.) for the studied complexes.*

Localized orbital locator (LOL, Figure 1) maps are often used to explain structures and bonds in a clear and intuitive way. The limit possible values of LOL are: upper limit LOL = 1 for perfect localization, upper limit LOL = 0.5 for gas-like electron pairs, and lower limit LOL = 0 for non-bonding regions. To make the image sharper, we set the color ratio from 0.0 to 0.8. Thus, the pale green LOL basins (LOL=0.3~0.6) represent fast-moving electrons (delocalized electrons). The slowest electron region is yellowish red (LOL=0.6~0.8), which conforms to the typical two-electron/two-center bonding situation.

The detailed description of transition density matrix (TDM) maps.

To describe intramolecular and intermolecular CTs more clearly, transition density matrix (TDM) maps have been performed, where a large value in diagonal term (bright area) corresponds to obvious intramolecular CT, and the bright area in off-diagonal term denotes that intermolecular CT.

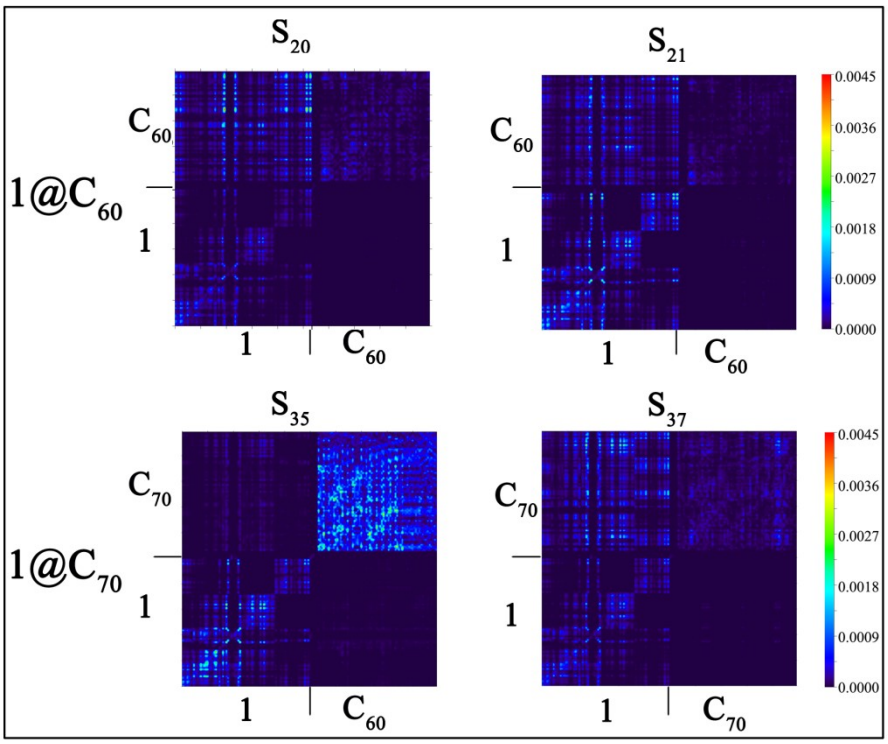

Figure S1. The TDM corresponding to the crucial electronic transitions of the complexes (The hydrogen atoms have been omitted).

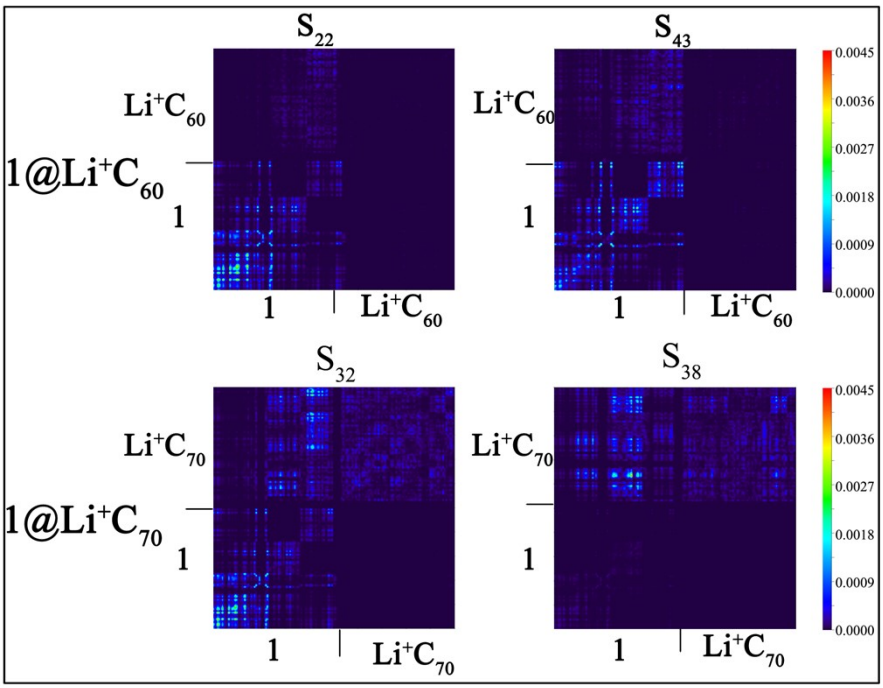

Figure S2. The TDM corresponding to the crucial electronic transitions of the complexes (The hydrogen atoms have been omitted).

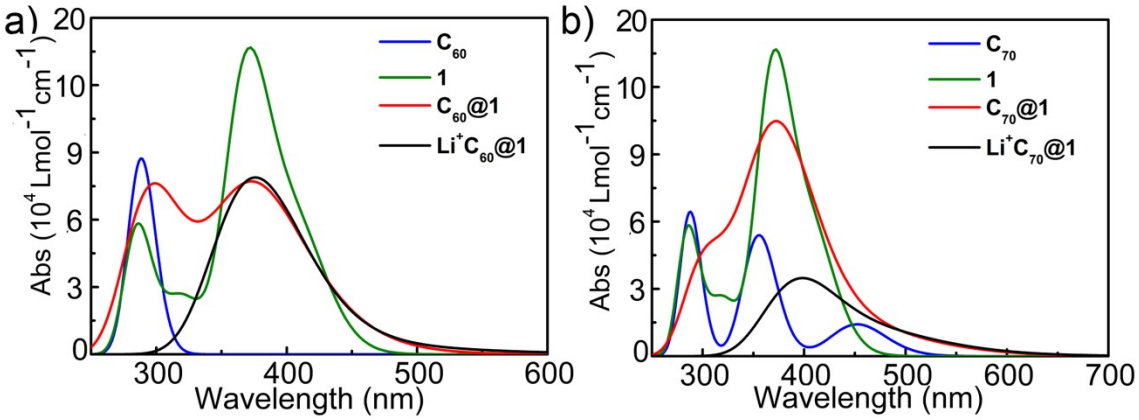

Figure S3. The comparison of absorption spectra of C_{60}, C_{70}, **1** and these four complexes calculated at the TD-CAM-B3LYP/6-31G (d). The spectral envelope was obtained by convolution of the stick spectra using Gaussian function of 0.6 eV FWHM.

Table S1. The components of the total polarizability α_{tot} (a.u.) for the studied complexes obtained by BhandHLYP/6-31+G(d) and CAM-B3LYP/6-31+G(d) level.

Complex	Functional	α_{xx}	α_{yy}	α_{zz}	α_{tot}
C_{60}@1	BHandHLYP	1854.9	1471.9	1141.4	1489.4
	CAM-B3LYP	1859.3	1472.0	1145.3	1492.2
C_{70}@1	BHandHLYP	2015.8	1580.1	1255.5	1617.1
	CAM-B3LYP	2020.2	1575.8	1258.7	1618.2
Li^+C_{60}@1	BHandHLYP	1909.1	1408.6	1134.2	1483.4
	CAM-B3LYP	1908.2	1407.8	1136.9	1484.3
Li^+C_{70}@1	BHandHLYP	2002.1	1580.1	1240.8	1607.6
	CAM-B3LYP	2003.5	1578.3	1242.2	1608.0

Table S2. The components of the first hyperpolarizability β (a.u.) and the projection of β on dipole moment (β_{vec}) for studied complexes obtained by BhandHLYP/6-31+G(d) and CAM-B3LYP/6-31+G(d) level.

Complex	Functional	β_x	β_{tot}	β_{vec}
C_{60}@1	BHandHLYP	3786.6	4078.3	3583.3
	CAM-B3LYP	3004.8	3264.1	2760.3
C_{70}@1	BHandHLYP	4127.7	4325.9	4256.0
	CAM-B3LYP	3315.1	3537.7	3462.7
Li^+C_{60}@1	BHandHLYP	5758.2	5772.3	5756.9
	CAM-B3LYP	5689.4	5121.3	5675.6
Li^+C_{70}@1	BHandHLYP	4525.6	5883.8	4721.1
	CAM-B3LYP	4368.3	5268.5	4537.0

Table S3. The components of second hyperpolarizability γ (a.u.) and for studied complexes obtained by CAM-B3LYP/6-31+G(d) level.

Complex	γ_{xxxx}	γ_{yyyy}	γ_{zzzz}	γ_{xxyy}	γ_{xxzz}	γ_{yyzz}
C_{60}@1	3438610	1319980	52996	721447	66173	83810
C_{70}@1	3246400	1017020	55118	1072680	47263	62806
Li^+C_{60}@1	3794760	1621490	56777	1077010	52251	99226
Li^+C_{70}@1	3879280	1905130	47791	1102010	41224	43412

Structures and energies of the complexes

C_{60}@1: energy = -5528.04 47359 au

C	3.65444900	3.16071600	-0.72347400
C	3.74067800	2.17543100	0.31236300
C	4.81849400	1.28528500	0.33361700
C	5.85079300	1.37170800	-0.62428200
C	5.83536300	2.41598700	-1.58271500
C	4.72884600	3.26764800	-1.63845600
C	7.01001400	0.45148000	-0.58127300
C	8.27485800	1.01635400	-0.92999300
C	8.32190600	2.38396200	-1.58431100
C	7.06068000	2.59279600	-2.45524000
C	6.91677100	-0.90977200	-0.15360700
C	8.10116400	-1.62694600	0.20628700
C	9.32571700	-1.00681100	-0.03629400
C	9.41110900	0.26531800	-0.63826600
C	5.65103500	-1.68463000	-0.17424500
C	5.51481500	-2.81357900	0.67540400
C	6.67085200	-3.16078300	1.58840100
C	7.98962900	-3.01842100	0.79879700
C	4.63728000	-1.40282700	-1.11689100
C	3.48647200	-2.19148600	-1.20455800
C	3.33164800	-3.32359500	-0.34068700
C	4.36407800	-3.60128200	0.58621100
O	2.73507700	2.18420900	1.23471500
C	2.79389200	1.20499800	2.27973000
O	2.47348700	-1.96931000	-2.08882200
C	2.52397700	-0.76851300	-2.87091200
C	2.18935100	-4.15411200	-0.44791400
C	2.52619500	4.01364000	-0.80769000
C	10.71535600	-1.49944100	0.20804100
N	11.56672900	-0.50151300	-0.30747900
C	10.85458900	0.60252000	-0.81964700
O	11.37512200	1.60452900	-1.29942200
O	11.10440400	-2.53525300	0.73867900
C	1.52101900	4.71374800	-0.88816700
C	1.18788300	-4.84829900	-0.60107000
C	-1.49639100	-5.73500700	2.80978200
C	-0.49406600	-5.65684500	1.83980800
C	-2.84243300	-6.16271900	2.48414400
C	-0.73764600	-6.01872200	0.45906200
C	-1.96445900	-6.63117300	0.21795300

C	-2.98882600	-6.69665200	1.20286400
C	-2.58482900	-6.65267800	-1.06019100
C	-4.23890000	-6.75236300	0.53073200
C	-4.09098000	-5.85576800	3.15776800
C	-3.98921800	-6.72881000	-0.86790100
C	-5.31999500	-5.90464000	2.49456200
C	-0.03375400	-5.55449700	-0.74029100
C	-5.42057000	-6.26602500	1.09324700
C	-0.65747100	-5.59933100	-2.01228200
C	-2.00902900	-6.06557800	-2.18963800
C	-6.45777500	-5.93965000	0.13291400
C	-6.21252600	-5.91962200	-1.24286100
C	-2.94678400	-5.75271600	-3.25389000
C	-4.90625200	-6.22591200	-1.79260700
C	-4.32827300	-5.82883400	-3.06276800
C	-5.93572600	6.30662500	0.73479300
C	-5.83884300	6.35022700	-0.65882000
C	-4.77622400	6.47293200	1.59150100
C	-4.57257200	6.56750600	-1.33283400
C	-3.52206300	6.92836900	-0.48794700
C	-3.62021100	6.88716100	0.92834300
C	-2.15886700	6.75133500	-0.83754100
C	-2.31625700	6.68995300	1.45533700
C	-4.55990000	6.01710300	2.95143000
C	-1.41292000	6.59904900	0.36176800
C	-3.27661700	5.82502100	3.47152100
C	-4.16720500	6.20909300	-2.67904000
C	-2.08247500	6.06681600	2.68190200
C	-2.82480700	6.03550200	-3.02598000
C	-1.75572300	6.20210300	-2.05678400
C	-0.75352600	5.50578900	2.83080800
C	0.13093500	5.40447100	1.75293400
C	-0.42841300	5.64019200	-2.05873500
C	-0.22719400	5.87536300	0.43159100
C	0.31749900	5.46379300	-0.86742600
C	13.02196200	-0.54274000	-0.18817800
C	13.48980800	-0.02500300	1.18285000
C	15.01666800	-0.11174100	1.38333900
C	15.77992100	0.76807000	0.37453200
C	15.37839900	0.28690300	2.82588700
H	4.87579200	0.50794900	1.08911400
H	4.68959400	4.05598200	-2.39078100
H	9.24511500	2.47966600	-2.16727000
H	8.35114700	3.16460600	-0.80398500

H	7.06955500	1.85264900	-3.27491100
H	7.06581100	3.59225600	-2.91245200
H	6.70076400	-2.47604300	2.45449700
H	6.56117300	-4.18221300	1.97893400
H	8.00089000	-3.76118900	-0.01839900
H	8.86673500	-3.22120300	1.42414800
H	4.76762400	-0.56349000	-1.79150200
H	4.26011400	-4.47680400	1.22801800
H	1.91210800	1.38502300	2.90242800
H	2.75022700	0.18424900	1.86647600
H	3.71463600	1.32249700	2.87570100
H	1.57710100	-0.73894900	-3.42037500
H	2.60697200	0.11974800	-2.22402100
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H	-6.20968000	-5.55583500	3.02200500
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H	15.60416200	0.45251300	-0.66425900
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C	-4.77075700	-0.48405000	-3.22034600
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C	-4.66434600	0.96701100	-3.18453600
C	-5.67048000	0.16140500	2.83815900
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C	-1.79259000	-2.31842000	-1.99758800
C	-1.45403700	2.28890400	-1.88521200
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C	-0.32232400	-1.60195500	0.34597200
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C	-0.88300800	2.48056900	0.51345200
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C	-0.13924100	-0.88050000	-0.84402600
C	-1.39789200	-1.57539700	2.44340900
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C	-0.02889100	0.56899400	-0.81026100

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C	-1.54702500	2.49681400	1.80663500
C	-0.11783200	1.24893600	0.41502600
C	-1.19063800	1.27577100	2.51261100
C	-0.31035600	0.50241200	1.64837800
C	-2.74547900	2.40077900	-2.54780400
C	-3.62756000	3.17138200	-1.68391400
C	-2.88159000	3.54101500	-0.49154200
C	-3.42539100	-1.02985200	-3.34294900
C	-2.48809100	0.08335000	-3.38448100
C	-6.58659200	1.73971600	-0.25287000
C	-5.64944100	2.85229200	-0.29343500
C	-3.52091600	3.55367200	0.75650100
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C	-2.84174300	3.02213800	1.92585200

C_{70}@1: energy = -5909.1740317 au

C	-3.95377000	3.08111500	0.81412600
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C	-5.01333500	1.12879400	-0.22015800
C	-6.05858300	1.16930600	0.72891400
C	-6.06836900	2.19647300	1.70792400
C	-5.01828700	3.11800000	1.74478200
C	-7.21230500	0.24023600	0.64060400
C	-8.48072700	0.76388900	1.04503300
C	-8.54886300	2.08936900	1.77857400
C	-7.27156700	2.29775300	2.62045500
C	-7.12261400	-1.07934100	0.09396700
C	-8.30620600	-1.77268500	-0.31060700
C	-9.53129100	-1.19641100	0.01807700
C	-9.61484300	0.02104500	0.72317700
C	-5.85622400	-1.84726100	0.01312900
C	-5.72089500	-2.86097500	-0.96999000
C	-6.89542800	-3.12079900	-1.88835500
C	-8.19089400	-3.09315400	-1.04793100
C	-4.83992600	-1.67648800	0.97739500
C	-3.68209700	-2.46093000	0.95931500
C	-3.51672700	-3.46071100	-0.05262800
C	-4.55603900	-3.63182900	-0.99787400
O	-2.94025600	2.07931000	-1.08480500
C	-2.84960300	0.99632600	-2.02110500
O	-2.67400900	-2.35350000	1.86960200
C	-2.79097100	-1.33026800	2.86684400

C	-2.36653400	-4.28882400	-0.08043300
C	-2.92366100	4.05340400	0.81595900
C	-10.91933700	-1.69579000	-0.21872400
N	-11.76841400	-0.75891800	0.40297300
C	-11.05806500	0.31498300	0.97741900
O	-11.58066600	1.26239400	1.55568500
O	-11.30780900	-2.69678900	-0.81284800
C	-2.01889600	4.88254400	0.76148100
C	-1.37928000	-5.01916800	-0.08198700
C	1.37537000	-5.14006200	-3.56383400
C	0.34991800	-5.24097600	-2.61907200
C	2.67158900	-5.75291400	-3.35138000
C	0.51856900	-5.97467700	-1.38184000
C	1.68819000	-6.72440200	-1.29648800
C	2.73448100	-6.61067400	-2.25193300
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C	3.96104600	-5.40759700	-3.92099400
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C	5.19082300	-6.44188400	-2.01833500
C	0.39521300	-6.20710300	1.11229900
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C	5.93905800	-6.78987100	0.33244300
C	2.63237600	-6.85588700	2.29122700
C	4.59339200	-7.09912600	0.77702000
C	4.00981700	-6.99622000	2.10114300
C	4.99433100	6.91637500	-1.92140400
C	5.00238900	7.26627200	-0.56833200
C	3.75900000	6.75883300	-2.66701000
C	3.77581100	7.49257300	0.17371000
C	2.62290000	7.53187800	-0.61187400
C	2.61461200	7.17943300	-1.98831200
C	1.32492500	7.29221600	-0.08936400
C	1.31073600	6.72233000	-2.31867200
C	3.49723300	5.98955900	-3.86973500
C	0.51452700	6.78625200	-1.14194500
C	2.21475800	5.54181900	-4.19617100
C	3.52830800	7.40834400	1.60183700
C	1.06754400	5.81520000	-3.35025000
C	2.25205600	7.17146100	2.11716600
C	1.09494400	6.99316300	1.25514000

C	-0.17803600	5.08077300	-3.22733000
C	-0.95304800	5.12858700	-2.06640300
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C	-13.79708800	-0.23031600	-0.92687200
C	-15.33033300	-0.35888500	-1.03520400
C	-16.05494500	0.40592700	0.08935800
C	-15.80231000	0.13876500	-2.41364600
H	-5.03448700	0.36616300	-0.99136600
H	-5.02582600	3.91323500	2.49071400
H	-9.45570500	2.12163700	2.39320300
H	-8.63144700	2.90869500	1.04275900
H	-7.23256900	1.52133500	3.40494900
H	-7.29296400	3.27476500	3.12331500
H	-6.96245400	-2.34256000	-2.66907400
H	-6.78189800	-4.08925300	-2.39533100
H	-8.16120500	-3.91893200	-0.31538100
H	-9.08448500	-3.24649600	-1.66388200
H	-4.97543400	-0.92535400	1.74842000
H	-4.44693800	-4.41619000	-1.74757500
H	-1.91301100	1.16021600	-2.56401500
H	-2.81349400	0.02797600	-1.49672000
H	-3.70327500	1.00531700	-2.71935100
H	-1.87603500	-1.39754800	3.46316600
H	-2.85832400	-0.33307400	2.40180500
H	-3.67576600	-1.49960000	3.50318700
H	1.22626600	-4.48441700	-4.42347800
H	-0.56293500	-4.66287200	-2.76595000
H	4.00012700	-4.77986800	-4.81297700
H	6.09300800	-5.35147600	-3.70611800
H	-0.12397600	-5.93778500	2.03243800
H	7.23321400	-6.14626000	-1.25114500
H	6.73745600	-6.69315200	1.07034400
H	2.26312600	-6.66975600	3.30117400
H	4.66435700	-6.91459500	2.97076500
H	5.94213300	6.65422800	-2.39531000
H	5.95587700	7.26316900	-0.03707000
H	4.33548000	5.65829400	-4.48537400
H	2.09996800	4.87619000	-5.05366700
H	4.37274300	7.42233400	2.29345000
H	2.14699900	7.00790300	3.19107400
H	-0.46300200	4.37764400	-4.01216000

H	-1.80804200	4.45930800	-1.96848800
H	-0.40234100	6.03016700	2.54729600
H	-13.49654500	-1.90275500	0.43495300
H	-13.59459300	-0.30801200	1.25006600
H	-13.51304600	0.83422500	-0.97278700
H	-13.32600300	-0.73845800	-1.78252100
H	-15.58621500	-1.43036400	-0.94864300
H	-17.14634300	0.32775100	-0.02858800
H	-15.79522000	0.01932900	1.08559300
H	-15.78440100	1.47380600	0.05845000
H	-16.89119500	0.02154100	-2.52396200
H	-15.30965700	-0.41598800	-3.22673400
H	-15.56229000	1.20749500	-2.53570400
C	6.95458800	-0.18022700	1.57553100
C	6.95223700	0.86495600	0.60262400
C	6.76138600	0.50716900	-0.81471600
C	6.58674100	-0.86926900	-1.15319400
C	6.68108200	-1.91516100	-0.15329100
C	6.86454900	-1.57558200	1.19216400
C	5.60768500	-1.27940300	-2.12957700
C	5.09984800	-2.57800900	-1.73362600
C	3.74731200	-2.88002300	-1.92057500
C	2.86477900	-1.89710800	-2.51476200
C	3.35596100	-0.64512800	-2.99542400
C	1.58725300	-1.99288500	-1.85221600
C	0.76569700	-0.84270500	-1.65575300
C	0.07547600	-0.68263200	-0.36166800
C	0.26479100	-1.68402300	0.63617000
C	1.03251500	-2.88131400	0.37293600
C	1.68446300	-3.03479600	-0.85203800
C	0.45438800	-1.33381300	2.02005800
C	1.33320100	-2.31996500	2.61453400
C	2.27887300	-1.92438400	3.56700700
C	2.37242900	-0.52869600	3.94844700
C	1.45740000	0.44692900	3.44736800
C	0.46002900	0.02810100	2.44619700
C	4.28095800	1.08184000	3.84161000
C	5.58693600	1.18084000	3.16516400
C	6.28129000	-0.02403900	2.84122900
C	5.77552100	-1.32322800	3.24070200
C	4.53443200	-1.41698800	3.88169100
C	3.76628200	-0.21527700	4.14346100
C	4.78108500	-0.32391100	-2.79531900
C	5.15973600	1.04632000	-2.65756000

C	2.41496700	0.42755700	-3.04366500
C	4.19421900	2.11869700	-2.79920900
C	2.84057000	1.81219000	-2.98756600
C	1.13621600	0.32955700	-2.38182600
C	0.77244100	1.65454500	-1.91795000
C	0.12409300	1.80406800	-0.68682500
C	-0.19073000	0.63734900	0.11151900
C	-0.00710600	0.98884500	1.49879500
C	0.42015600	2.37299400	1.55388800
C	1.36801700	2.77228000	2.50328600
C	1.92112600	1.79682800	3.42249500
C	3.31591000	2.11025400	3.61746800
C	3.62540100	3.27929900	2.81836600
C	4.86687600	3.37536600	2.17718700
C	5.83162200	2.30162000	2.31489800
C	6.50604600	2.14582400	1.04958200
C	5.95804600	3.12331300	0.12930800
C	5.77557600	2.78251200	-1.21658900
C	6.13779500	1.45684600	-1.67951500
C	1.82160300	2.58005700	-2.30010400
C	0.49294100	2.88508900	0.20071900
C	2.41930900	3.70098700	2.13263300
C	4.94773900	3.89805100	0.82634700
C	4.57645500	3.20409000	-1.91603000
C	5.77095700	-2.98585200	-0.51538700
C	3.01657800	-3.60315100	-0.89984400
C	1.68618900	-3.29287400	1.59829500
C	3.61670100	-2.48685700	3.53542700
C	6.14437600	-2.29469300	2.22696800
C	3.65895100	-3.99555000	0.28459500
C	2.98103500	-3.83281600	1.55919900
C	3.96507600	-3.42284000	2.54598000
C	5.25424100	-3.32733600	1.87957900
C	5.06243400	-3.67718800	0.48193600
C	3.77898000	4.29511400	0.15575600
C	2.49349900	4.19256000	0.82018900
C	1.51176400	3.77707800	-0.16325000
C	2.19007100	3.62179900	-1.43524500
C	3.59078600	3.94174200	-1.23976100

Li^+C_{60}@1: energy = -5535.3799072 au

C	3.66517000	3.16073200	-0.72331900
C	3.75142200	2.17544600	0.31251600
C	4.82923100	1.28529100	0.33373800
C	5.86150200	1.37170500	-0.62419300
C	5.84605200	2.41598400	-1.58262500
C	4.73954100	3.26765500	-1.63833400
C	7.02071600	0.45146800	-0.58121800
C	8.28555500	1.01633000	-0.92997600
C	8.33259400	2.38393700	-1.58429600
C	7.07134500	2.59278200	-2.45518700
C	6.92747400	-0.90978400	-0.15354800
C	8.11187200	-1.62696800	0.20631100
C	9.33642300	-1.00684400	-0.03630800
C	9.42180800	0.26528400	-0.63828300
C	5.66173100	-1.68463100	-0.17414800
C	5.52552700	-2.81357800	0.67550500
C	6.68158800	-3.16079200	1.58846800
C	8.00034300	-3.01844200	0.79882400
C	4.64795000	-1.40282000	-1.11676300
C	3.49713300	-2.19146900	-1.20439600
C	3.34232500	-3.32357600	-0.34052000
C	4.37478000	-3.60127100	0.58634700
O	2.74584900	2.18423300	1.23489800
C	2.80468600	1.20502200	2.27991200
O	2.48412300	-1.96928500	-2.08862900
C	2.53460000	-0.76848800	-2.87072200
C	2.20001800	-4.15408300	-0.44771200
C	2.53692100	4.01366600	-0.80750100
C	10.72606500	-1.49948500	0.20798600
N	11.57743100	-0.50156500	-0.30756000
C	10.86528500	0.60247400	-0.81970700
O	11.38581300	1.60447900	-1.29949800
O	11.11512000	-2.53530000	0.73861200
C	1.53174900	4.71378200	-0.88794900
C	1.19853900	-4.84826100	-0.60083800
C	-1.48564000	-5.73494500	2.81009500
C	-0.48334400	-5.65679300	1.84009100
C	-2.83169600	-6.16264600	2.48449800
C	-0.72696800	-6.01866800	0.45935200
C	-1.95379400	-6.63110800	0.21828100
C	-2.97813200	-6.69657800	1.20322200
C	-2.57420200	-6.65260800	-1.05984500

C	-4.22822700	-6.75227900	0.53112800
C	-4.08022000	-5.85568300	3.15815900
C	-3.97858600	-6.72872800	-0.86751300
C	-5.30925500	-5.90454600	2.49499000
C	-0.02310800	-5.55444900	-0.74002200
C	-5.40987500	-6.26593000	1.09367800
C	-0.64686400	-5.59927800	-2.01199400
C	-1.99843100	-6.06551400	-2.18930900
C	-6.44710700	-5.93954700	0.13337600
C	-6.20189900	-5.91952100	-1.24240700
C	-2.93621600	-5.75264400	-3.25353400
C	-4.89564400	-6.22582300	-1.79219200
C	-4.31770000	-5.82875000	-3.06237100
C	-5.92493300	6.30672500	0.73523500
C	-5.82809300	6.35032500	-0.65838100
C	-4.76540500	6.47302200	1.59190700
C	-4.56183900	6.56759300	-1.33243300
C	-3.51130200	6.92844700	-0.48757700
C	-3.60940800	6.88724100	0.92871500
C	-2.14811800	6.75140100	-0.83721200
C	-2.30544000	6.69002100	1.45567100
C	-4.54904300	6.01719100	2.95183000
C	-1.40213700	6.59910900	0.36207400
C	-3.26574700	5.82509800	3.47188400
C	-4.15651600	6.20917600	-2.67865100
C	-2.07162700	6.06688300	2.68222800
C	-2.81413000	6.03557300	-3.02563100
C	-1.74501500	6.20216600	-2.05646800
C	-0.74267700	5.50584400	2.83109500
C	0.14175000	5.40451800	1.75319400
C	-0.41771000	5.64024200	-2.05845900
C	-0.21641400	5.87541300	0.43186100
C	0.32823600	5.46383800	-0.86717100
C	13.03266700	-0.54280500	-0.18830200
C	13.50055900	-0.02507100	1.18271100
C	15.02742400	-0.11182200	1.38315500
C	15.79065500	0.76798200	0.37432400
C	15.38920200	0.28681900	2.82569100
H	4.88654500	0.50795600	1.08923300
H	4.70027300	4.05598900	-2.39065700
H	9.25578700	2.47963400	-2.16728300
H	8.36186600	3.16458100	-0.80397100
H	7.08018800	1.85263500	-3.27485800
H	7.07647000	3.59224200	-2.91240000

H	6.71153200	-2.47605200	2.45456200
H	6.57191200	-4.18222100	1.97900500
H	8.01157300	-3.76121000	-0.01837200
H	8.87746500	-3.22123100	1.42414900
H	4.77828100	-0.56348400	-1.79137900
H	4.27082800	-4.47679300	1.22815800
H	1.92292200	1.38505600	2.90263600
H	2.76100000	0.18427400	1.86666000
H	3.72545000	1.32251300	2.87585500
H	1.58770800	-0.73891600	-3.42015600
H	2.61762200	0.11977300	-2.22383300
H	3.38293500	-0.79069200	-3.57522600
H	-1.27325400	-5.34623300	3.80770400
H	0.47574400	-5.20982800	2.10404300
H	-4.05565600	-5.47172500	4.17954900
H	-6.19892200	-5.55573200	3.02245900
H	-0.12146200	-5.12879700	-2.84357600
H	-7.41773800	-5.59333200	0.49260600
H	-6.99090700	-5.56015300	-1.90545600
H	-2.56138300	-5.33949100	-4.19143600
H	-4.97230500	-5.47241300	-3.85966700
H	-6.88247000	6.03024500	1.18012400
H	-6.71453500	6.11006000	-1.24814900
H	-5.40508300	5.71264000	3.55668000
H	-3.16979700	5.37839200	4.46317100
H	-4.91935000	5.95900500	-3.41802700
H	-2.57832300	5.65884100	-4.02230900
H	-0.46369100	5.03595400	3.77591700
H	1.07557600	4.85560800	1.87954200
H	-0.01219400	5.20767700	-2.97367500
H	13.34471800	-1.58707400	-0.32829700
H	13.43331100	0.07221900	-1.00301300
H	13.17545300	1.02256100	1.29541100
H	12.99525100	-0.61687500	1.96160100
H	15.32962000	-1.16325600	1.22869700
H	16.87425300	0.72425700	0.56168100
H	15.61486200	0.45242600	-0.66446200
H	15.47008100	1.81816700	0.46861600
H	16.47268900	0.20102700	2.99930800
H	14.86889900	-0.35083000	3.55672900
H	15.09680100	1.33230800	3.01650100
C	-6.78460800	-1.11282400	-0.32291300
C	-6.59489800	-0.36610900	-1.55909400
C	-6.49221800	1.03496200	-1.52419400

C	-6.76135500	1.01926100	0.93973500
C	-6.86730200	-0.43234400	0.90385100
C	-5.71246100	-1.13934900	-2.42111400
C	-5.50351500	1.71334800	-2.35016000
C	-6.01446800	1.38602500	2.13458700
C	-6.18580600	-0.96211800	2.07646800
C	-6.02133600	-2.34814300	-0.42150500
C	-5.10930400	2.46027600	2.09355400
C	-4.91688000	3.20348400	0.85837100
C	-4.76014200	-0.48396200	-3.21993700
C	-4.97654900	2.83705400	-1.58886900
C	-4.65371700	0.96709700	-3.18413100
C	-5.65967700	0.16150200	2.83859500
C	-5.44747700	-2.15392300	1.98011200
C	-5.36144500	-2.85612900	0.70898800
C	-5.35833600	-2.36518900	-1.71811600
C	-4.15487500	-2.26347600	2.64132100
C	-4.01869100	-3.40035600	0.58523200
C	-4.06044500	-2.88582100	-1.83311800
C	-4.41261300	0.05433300	3.47777700
C	-3.24291900	1.31759800	-3.28430500
C	-3.27427900	-3.03280100	1.77723100
C	-3.37972700	-3.41608300	-0.66238700
C	-3.07270300	-2.20932000	-2.66075800
C	-1.78195500	-2.31835700	-1.99726800
C	-1.44335800	2.28896400	-1.88490300
C	-1.97571500	-3.05892700	-0.76189800
C	-1.25446700	-2.70776300	0.38649600
C	-0.31161100	-1.60190400	0.34624800
C	-1.91652000	-2.69386300	1.67964500
C	-3.47543200	1.16851100	3.43771800
C	-0.70167500	1.10004400	-1.98263600
C	-3.64748600	-1.18086800	3.37939500
C	-2.23748500	-0.82993900	3.27788600
C	-1.22979200	-0.02360500	-2.74308200
C	-1.53152000	2.98889400	-0.61388200
C	-0.87225600	2.48062500	0.51374300
C	-0.87446800	-1.24750200	-2.03879300
C	-0.12855800	-0.88045100	-0.84375500
C	-1.38711600	-1.57533600	2.44371700
C	-0.39744700	-0.89813500	1.61648500
C	-0.01819500	0.56904200	-0.80999500
C	-2.13151200	0.62177700	3.31369200
C	-1.53623400	2.49687500	1.80694600

C	-0.10709300	1.24898500	0.41529500
C	-1.17983600	1.27583000	2.51291200
C	-0.29958700	0.50246300	1.64865400
C	-2.73481900	2.40084900	-2.54745600
C	-3.61686700	3.17146000	-1.68354000
C	-2.87085900	3.54108800	-0.49119100
C	-3.41478500	-1.02977600	-3.34258000
C	-2.47747600	0.08341800	-3.38414100
C	-6.57586900	1.73982000	-0.25240700
C	-5.63870900	2.85238900	-0.29300000
C	-3.51014700	3.55375100	0.75687100
C	-3.81684800	2.34765500	2.75465000
C	-2.83094300	3.02221100	1.92620200
Li	-3.20043500	-0.01428000	-0.07942000

Li^+C_{70}@1: energy = -5535.3799072 au

C	-3.96339700	3.08087900	0.81412600
C	-3.98041600	2.05811200	-0.18890600
C	-5.02358900	1.12889800	-0.22015800
C	-6.06882400	1.16974600	0.72891400
C	-6.07828000	2.19691600	1.70792400
C	-5.02790200	3.11810500	1.74478200
C	-7.22284400	0.24104600	0.64060400
C	-8.49109800	0.76510600	1.04503300
C	-8.55880800	2.09060800	1.77857400
C	-7.28144500	2.29858200	2.62045500
C	-7.13357700	-1.07856000	0.09396700
C	-8.31739100	-1.77152400	-0.31060700
C	-9.54229100	-1.19485600	0.01807700
C	-9.62545200	0.02262700	0.72317700
C	-5.86743300	-1.84688600	0.01312900
C	-5.73243000	-2.86064400	-0.96999000
C	-6.90704600	-3.12009100	-1.88835500
C	-8.20250300	-3.09203000	-1.04793100
C	-4.85108100	-1.67644000	0.97739500
C	-3.69350300	-2.46125300	0.95931500
C	-3.52845500	-3.46108700	-0.05262800
C	-4.56782100	-3.63187200	-0.99787400
O	-2.95020500	2.07874800	-1.08480500
C	-2.85989900	0.99573500	-2.02110500
O	-2.68538100	-2.35414700	1.86960200
C	-2.80201400	-1.33087800	2.86684400
C	-2.37852700	-4.28957000	-0.08043300
C	-2.93297600	4.05283700	0.81595900

C	-10.93049700	-1.69378900	-0.21872400
N	-11.77927400	-0.75664500	0.40297300
C	-11.06858000	0.31702800	0.97741900
O	-11.59087600	1.26460700	1.55568500
O	-11.31929100	-2.69466400	-0.81284800
C	-2.02794400	4.88168600	0.76148100
C	-1.39150800	-5.02023100	-0.08198700
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C	0.33761900	-5.24259400	-2.61907200
C	2.65912500	-5.75527800	-3.35138000
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C	2.72174200	-6.61305800	-2.25193300
C	2.25277900	-7.12889000	-0.06186700
C	3.94221800	-6.94519300	-1.60708000
C	3.94869300	-5.41037500	-3.92099400
C	3.65230300	-7.26269100	-0.25363500
C	5.14920600	-5.73809600	-3.28554200
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C	5.17813800	-6.44505600	-2.01833500
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C	1.69022200	-6.81081100	1.17551400
C	6.21093000	-6.47991800	-1.00020600
C	5.92626100	-6.79328400	0.33244300
C	2.61955800	-6.85823800	2.29122700
C	4.58049600	-7.10210700	0.77702000
C	3.99695400	-6.99901300	2.10114300
C	4.98593500	6.91326500	-1.92140400
C	4.99410600	7.26315900	-0.56833200
C	3.75055400	6.75612000	-2.66701000
C	3.76760000	7.48985400	0.17371000
C	2.61470200	7.52952900	-0.61187400
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C	1.31665000	7.29028400	-0.08936400
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C	3.52007000	7.40570500	1.60183700
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C	4.52336000	-1.41995000	3.88169100
C	3.75559600	-0.21799200	4.14346100
C	4.77036400	-0.32695200	-2.79531900
C	5.14945500	1.04315700	-2.65756000
C	2.40448800	0.42527600	-3.04366500
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C	1.91108600	1.79470500	3.42249500
C	3.30597100	2.10768300	3.61746800
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C	5.82174400	2.29824100	2.31489800
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C	3.64705100	-3.99823100	0.28459500
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C	3.95336000	-3.42561900	2.54598000
C	5.24255600	-3.33052900	1.87957900
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