

**Dehydrogenation of Ammonia-Borane to functionalize neutral and Li⁺-encapsulated
C₆₀, C₇₀ and C₃₆ fullerene cages: A DFT approach**

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Table S1 M06-2X/6-31G(d) calculated WBI values of concerned C-C and B-N (wherever applicable) bonds in the initial adduct and hydrogenated end products (neutral).

Complex	Bond Connectivity									
	C ₆₀			C ₇₀			C ₃₆			
	(6-5)	(6-6)	B-N	(6-5)	(6-6)	B-N	(6-5)	(6-6)	(5-5)	B-N
Adduct	1	1.17	0.62	1	1.16	0.63	1.08	1.01	0.93	0.63
(6-6) Product	-	0.79	-	-	0.79	-	-	0.79	-	-
(6-5) Product	0.77	-	-	0.77	-	-	0.78	-	-	-
(5-5) Product	-	-	-	-	-	-	-	-	0.78	-

Table S2 M06-2X/6-31G(d) calculated WBI values of concerned C-C and B-N (wherever applicable) bonds in the initial adduct, intermediate and hydrogenated end products (Li⁺-encapsulated).

System	Complex	Bond Connectivity			
		(6-5)	(6-6)	(5-5)	B-N
Li@C ₆₀	<i>Li@C₆₀^{AB}</i>	0.99	1.16	-	0.62
	<i>Li@C₆₀⁶⁻⁵</i>	0.76	-	-	-
	<i>Li@C₆₀⁶⁻⁶₁</i>	0.89	0.93	-	0.65
	<i>Li@C₆₀⁶⁻⁶</i>	-	0.79	-	-
Li@C ₇₀	<i>Li@C₇₀^{AB}</i>	1.01	1.12	-	0.63
	<i>Li@C₇₀⁶⁻⁵</i>	0.76	-	-	-
	<i>Li@C₇₀⁶⁻⁶₁</i>	0.91	0.91	-	0.64
	<i>Li@C₇₀⁶⁻⁶</i>	-	0.79	-	-
Li@C ₃₆	<i>Li@C₃₆^{AB}</i>	1.08	1.01	0.92	0.64
	<i>Li@C₃₆⁶⁻⁶₁</i>	0.86	0.86	-	0.63
	<i>Li@C₃₆⁶⁻⁶</i>	-	0.79	-	-
	<i>Li@C₃₆⁶⁻⁵₁</i>	0.88	0.85	-	0.64
	<i>Li@C₃₆⁶⁻⁵</i>	0.78	-	-	-
	<i>Li@C₃₆⁵⁻⁵₁</i>	0.85	-	0.85	0.63
	<i>Li@C₃₆⁵⁻⁵</i>	-	-	0.78	-

Table S3 TST calculated Rate constant values (k) (in sec⁻¹) of (6-6) & (6-5) hydrogenation reaction for the neutral fullerene systems at a temperature range of 100 K – 1000 K.

T (K)	C ₆₀		C ₇₀		C ₃₆	
	(6-6)	(6-5)	(6-6)	(6-5)	(6-6)	(6-5)
100	7.88x10 ⁻²²	2.79x10 ⁻⁴⁷	1.34x10 ⁻²³	1.30x10 ⁻³²	4.10x10 ⁻⁴¹	2.67x10 ⁻⁰⁴
200	6.46x10 ⁻⁰⁶	1.08x10 ⁻¹⁸	6.28x10 ⁻⁰⁷	1.97x10 ⁻¹¹	2.64x10 ⁻¹⁵	5.84x10 ⁺⁰³
300	1.13x10 ⁺⁰⁰	3.11x10 ⁻⁰⁹	1.92x10 ⁻⁰¹	1.85x10 ⁻⁰⁴	1.01x10 ⁻⁰⁶	1.51x10 ⁺⁰⁶
400	4.55x10 ⁺⁰²	1.60x10 ⁻⁰⁴	1.02x10 ⁺⁰²	5.30x10 ⁻⁰¹	1.99x10 ⁻⁰²	2.40x10 ⁺⁰⁷
500	1.65x10 ⁺⁰⁴	1.08x10 ⁻⁰¹	4.32x10 ⁺⁰³	6.19x10 ⁺⁰¹	7.55x10 ⁺⁰⁰	1.26x10 ⁺⁰⁸
600	1.82x10 ⁺⁰⁵	8.35x10 ⁺⁰⁰	5.29x10 ⁺⁰⁴	1.48x10 ⁺⁰³	4.01x10 ⁺⁰²	3.82x10 ⁺⁰⁸
700	1.02x10 ⁺⁰⁶	1.90x10 ⁺⁰²	3.19x10 ⁺⁰⁵	1.44x10 ⁺⁰⁴	6.93x10 ⁺⁰³	8.50x10 ⁺⁰⁸
800	3.75x10 ⁺⁰⁶	2.00x10 ⁺⁰³	1.23x10 ⁺⁰⁶	7.97x10 ⁺⁰⁴	5.94x10 ⁺⁰⁴	1.56x10 ⁺⁰⁹
900	1.04x10 ⁺⁰⁷	1.26x10 ⁺⁰⁴	3.57x10 ⁺⁰⁶	3.04x10 ⁺⁰⁵	3.18x10 ⁺⁰⁵	2.50x10 ⁺⁰⁹
1000	2.36x10 ⁺⁰⁷	5.54x10 ⁺⁰⁴	8.38x10 ⁺⁰⁶	8.94x10 ⁺⁰⁵	1.23x10 ⁺⁰⁶	3.67x10 ⁺⁰⁹

Table S4 Rate constant values (k) (in sec⁻¹) of Li@C₃₆–hydrogenation (Rate Determining Steps; r.d.s) at a temperature range of 100 K – 1000 K.

T (K)	Li@C ₃₆		
	(6-6)	(6-5)	(5-5)
100	1.55x10 ⁻⁹⁹	5.70x10 ⁻⁴⁵	5.14x10 ⁻⁶⁰
200	5.03x10 ⁻⁴³	4.20x10 ⁻¹⁶	1.51x10 ⁻²⁴
300	4.97x10 ⁻²⁴	2.05x10 ⁻⁰⁶	9.38x10 ⁻¹³
400	1.82x10 ⁻¹⁴	1.53x10 ⁻⁰¹	7.43x10 ⁻⁰⁷
500	1.09x10 ⁻⁰⁸	1.34x10 ⁺⁰²	2.62x10 ⁻⁰³
600	8.09x10 ⁻⁰⁵	1.25x10 ⁺⁰⁴	6.18x10 ⁻⁰¹
700	4.89x10 ⁻⁰²	3.26x10 ⁺⁰⁵	3.11x10 ⁺⁰¹
800	6.11x10 ⁺⁰⁰	3.81x10 ⁺⁰⁶	5.96x10 ⁺⁰²
900	2.66x10 ⁺⁰²	2.60x10 ⁺⁰⁷	5.99x10 ⁺⁰³
1000	5.51x10 ⁺⁰³	1.22x10 ⁺⁰⁸	3.82x10 ⁺⁰⁴

Table S5 Rate constant values (k) (in sec⁻¹) of Li@C₆₀-hydrogenation procedure [r.d.s for (6-6) & (6-5) hydrogenation along with (6-5)_Single Step addition] at a temperature range of 100 K – 1000 K.

T(K)	Li@C ₆₀		
	(6-6)	(6-5)	(6-5)_Single
100	4.82x10 ⁻¹⁶	1.66x10 ⁻³⁹	3.56x10 ⁻³⁵
200	1.75x10 ⁻⁰²	1.47x10 ⁻¹³	3.55x10 ⁻¹²
300	5.70x10 ⁺⁰²	7.80x10 ⁻⁰⁵	1.51x10 ⁻⁰⁴
400	1.04x10 ⁺⁰⁵	1.95x10 ⁺⁰⁰	9.76x10 ⁻⁰¹
500	2.39x10 ⁺⁰⁶	8.92x10 ⁺⁰²	1.92x10 ⁺⁰²
600	1.96x10 ⁺⁰⁷	5.47x10 ⁺⁰⁴	6.62x10 ⁺⁰³
700	8.88x10 ⁺⁰⁷	1.06x10 ⁺⁰⁶	8.44x10 ⁺⁰⁴
800	2.78x10 ⁺⁰⁸	9.90x10 ⁺⁰⁶	5.77x10 ⁺⁰⁵
900	6.80x10 ⁺⁰⁸	5.71x10 ⁺⁰⁷	2.60x10 ⁺⁰⁶
1000	1.40x10 ⁺⁰⁹	2.34x10 ⁺⁰⁸	8.76x10 ⁺⁰⁶

Table S6 Rate constant values (k) (in sec⁻¹) of Li@C₇₀-hydrogenation [r.d.s for (6-6) & (6-5) hydrogenation along with (6-5)_Single Step addition] at a temperature range of 100 K – 1000 K.

T (K)	Li@C ₇₀		
	(6-6)	(6-5)	(6-5)_Single
100	6.51x10 ⁻¹⁹	2.89x10 ⁻⁴⁹	4.61x10 ⁻²⁴
200	2.46x10 ⁻⁰⁴	4.61x10 ⁻¹⁸	3.56x10 ⁻⁰⁷
300	1.69x10 ⁺⁰¹	1.27x10 ⁻⁰⁷	1.25x10 ⁻⁰¹
400	4.44x10 ⁺⁰³	2.14x10 ⁻⁰²	6.98x10 ⁺⁰¹
500	1.27x10 ⁺⁰⁵	2.90x10 ⁺⁰¹	3.06x10 ⁺⁰³
600	1.20x10 ⁺⁰⁶	3.53x10 ⁺⁰³	3.81x10 ⁺⁰⁴
700	5.99x10 ⁺⁰⁶	1.08x10 ⁺⁰⁵	2.32x10 ⁺⁰⁵
800	2.02x10 ⁺⁰⁷	1.40x10 ⁺⁰⁶	9.02x10 ⁺⁰⁵
900	5.23x10 ⁺⁰⁷	1.02x10 ⁺⁰⁷	2.61x10 ⁺⁰⁶
1000	1.12x10 ⁺⁰⁸	5.01x10 ⁺⁰⁷	6.15x10 ⁺⁰⁶

Table S7 AIM analysis of all the initial adduct complexes, in course of hydrogenation procedure at M06-2X/6-31G(d) level.

System	BCP	$\rho(\mathbf{r})$	$\nabla^2\rho$	G	V	H	-G/V
C ₆₀	C-H(B)	0.0061	0.0193	0.0039	-0.0029	0.0010	1.3277
	C-H(N)	0.0109	0.0358	0.0077	-0.0064	0.0013	1.1974
C ₇₀	C-H(B)	0.0066	0.0196	0.0039	-0.0028	0.0010	1.3657
	C-H(N)	0.0106	0.0348	0.0074	-0.0062	0.0012	1.2016
C ₃₆	C-H(B)	0.0059	0.0169	0.0033	-0.0024	0.0009	1.3748
	C-H(B)	0.0057	0.0169	0.0033	-0.0024	0.0009	1.3922
	C-H(N)	0.0133	0.0394	0.0090	-0.0082	0.0008	1.0987
Li@C ₆₀	C-H(B)	0.0089	0.0301	0.0061	-0.0047	0.0014	1.3060
	C-H(B)	0.0090	0.0303	0.0061	-0.0047	0.0014	1.3070
Li@C ₇₀	C-H(B)	0.0085	0.0299	0.0061	-0.0048	0.0013	1.2754
Li@C ₃₆	C-H(B)	0.0097	0.0310	0.0062	-0.0047	0.0015	1.3203
	C-H(B)	0.0091	0.0307	0.0062	-0.0048	0.0015	1.3062

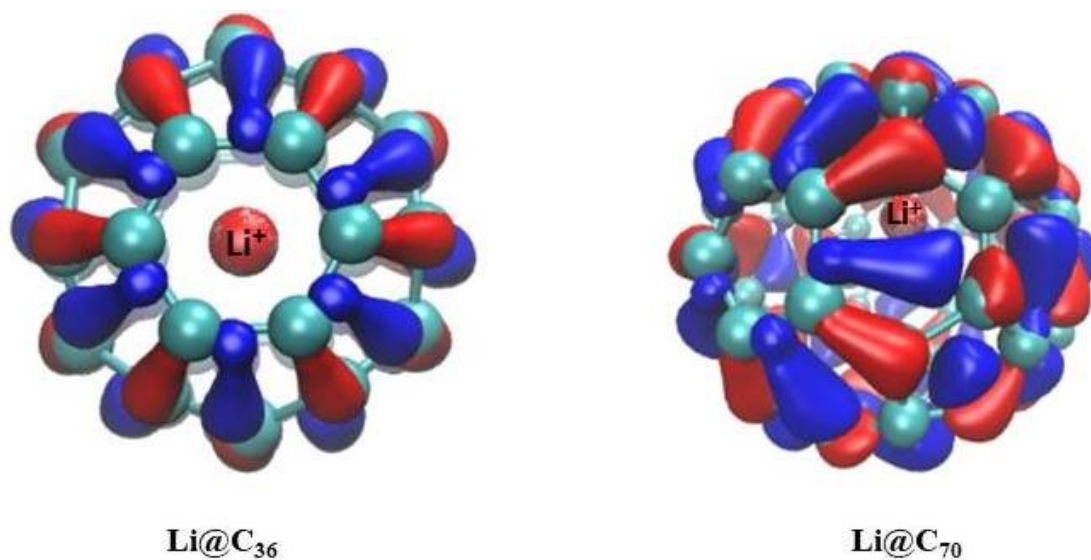


Fig. S1 Difference map of electron density corresponding to Li@C_{36} & Li@C_{70} , calculated at M06-2X/6-31G(d) level, where red and blue iso-surfaces (+0.13 and -0.13 a.u., respectively) represent the region in which electron density is increased and decreased after Li^+ confinement within the fullerene cages.

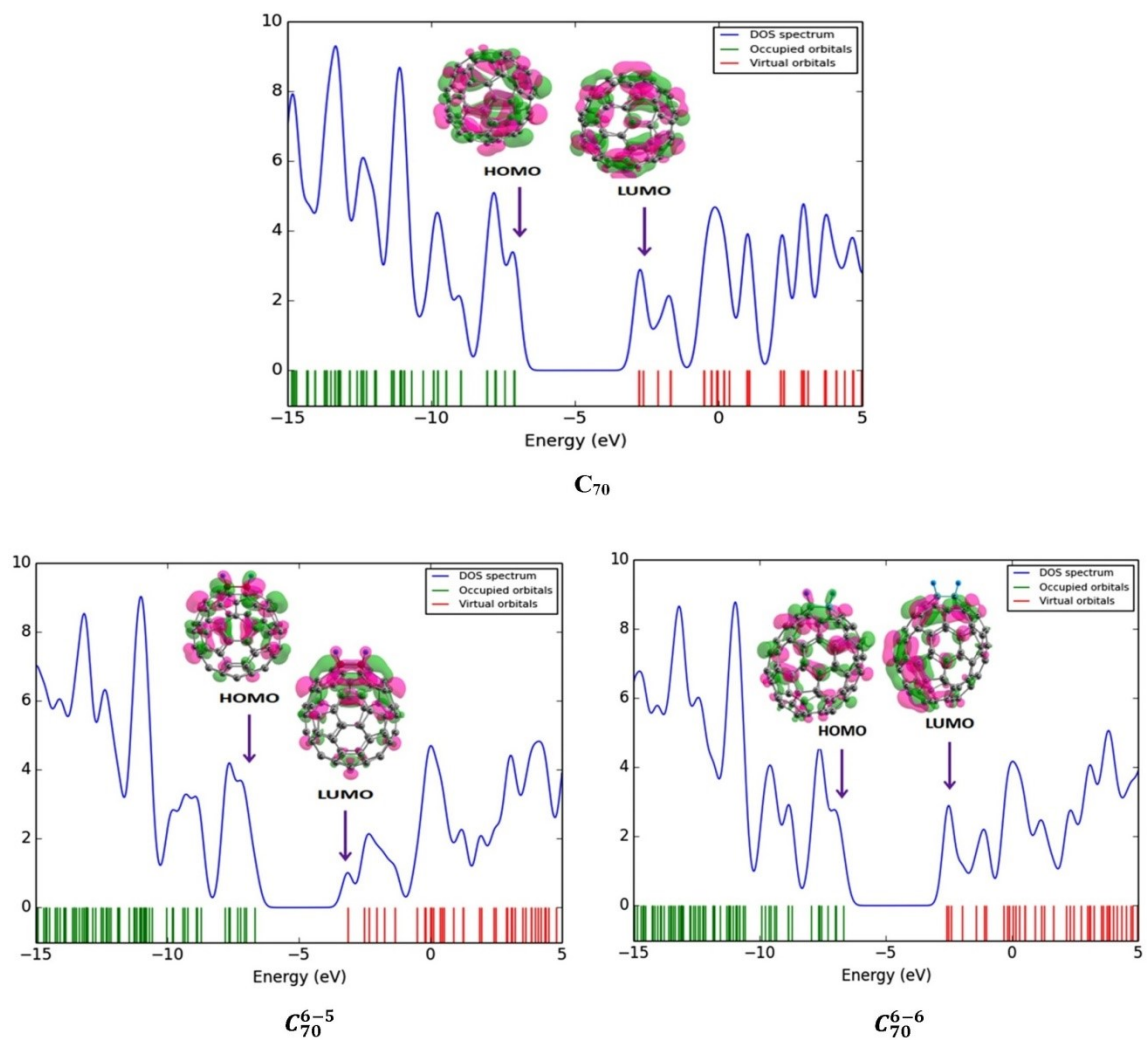


Fig.S2 HOMO-LUMO distribution along with Density of States (DOS) of pristine C_{70} & its hydrogenated products.

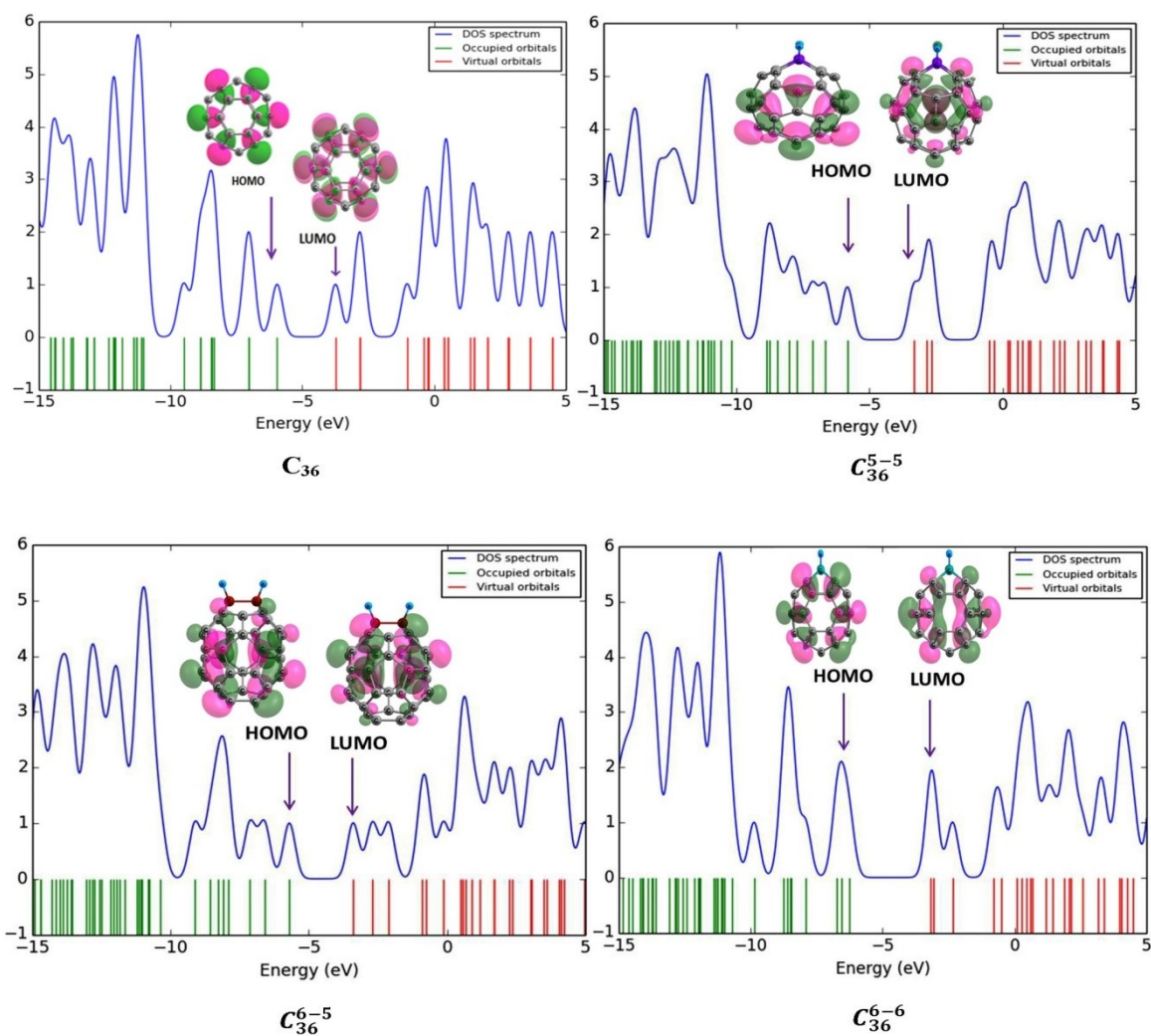


Fig.S3 HOMO-LUMO distribution along with Density of States (DOS) of pristine C_{36} & its hydrogenated products.

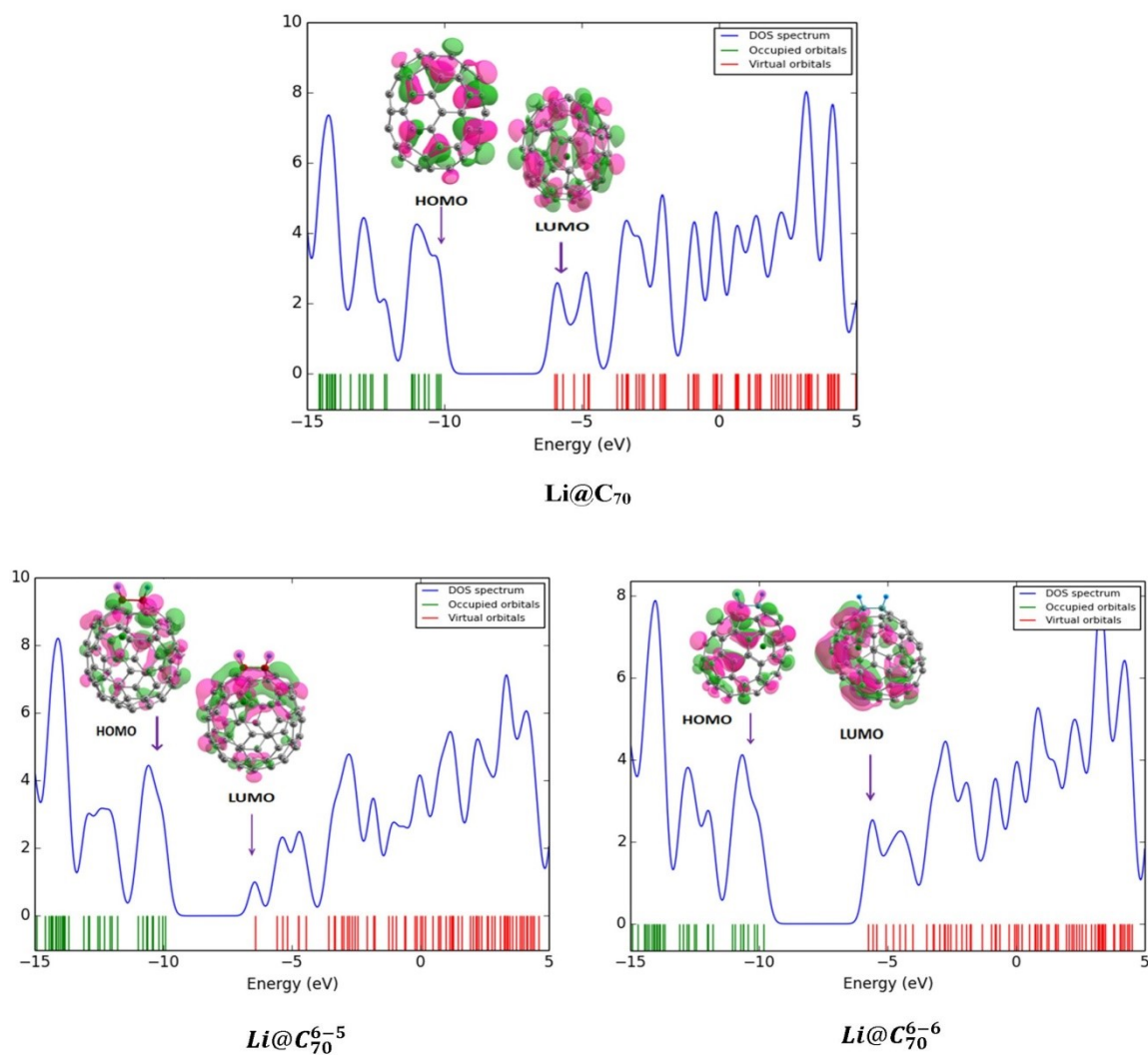


Fig.S4 HOMO-LUMO distribution along with Density of States (DOS) of Li@C_{70} & its hydrogenated products.

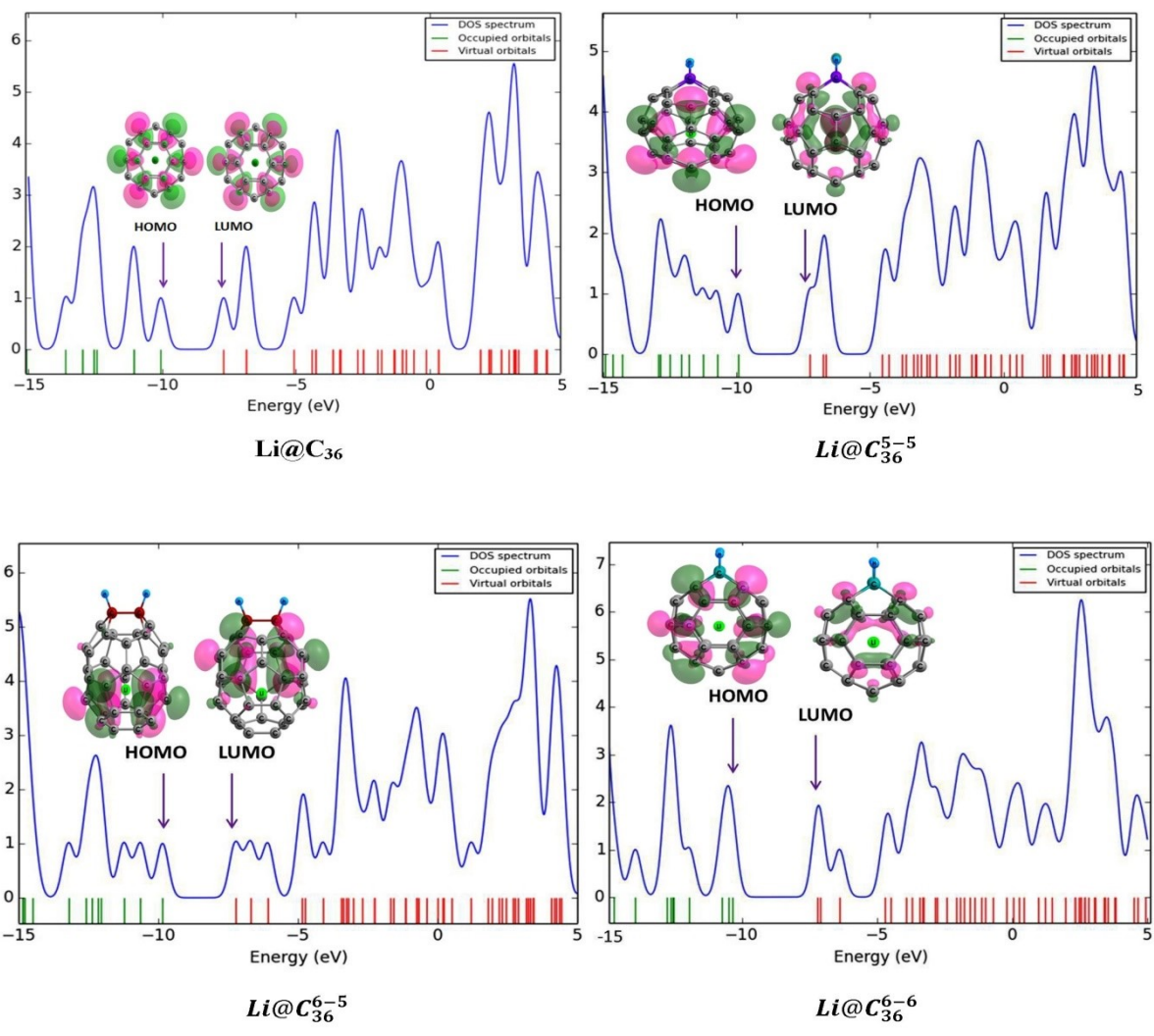


Fig.S5 HOMO-LUMO distribution along with Density of States (DOS) of Li@C_{36} & its hydrogenated products.

xyz coordinates of all reactants, TSs and products involved in the entire hydrogenation procedure:

C₆₀

0 1

C	-1.47313400	-2.98371700	-1.20656900
C	-1.94027600	-2.00826900	-2.17474200
C	-1.04594500	-1.43014600	-3.06373000
C	0.35703900	-1.80071400	-3.02580500
C	0.80393000	-2.73299400	-2.10080400
C	-0.13201900	-3.33746200	-1.17037000
C	-2.20152100	-2.77187500	0.03059900
C	-3.11842000	-1.66532300	-0.17260900
C	-2.95728800	-1.19371700	-1.53600600
C	-3.03542800	0.16336200	-1.81428300
C	-1.12727700	-0.01060300	-3.35443000
C	1.14243300	-0.60990600	-3.29321500
C	2.34001400	-0.40423700	-2.62455500
C	2.80814700	-1.37946000	-1.65654800
C	2.05724000	-2.51762800	-1.40041600
C	1.89525000	-2.98879900	-0.03741900
C	0.54223500	-3.49564500	0.10439400
C	-0.15388600	-3.29302100	1.28721800
C	-1.55670300	-2.92319800	1.24983000
C	-3.35033400	-0.75922300	0.85188400
C	-2.67625500	-0.91759000	2.12741600
C	-1.79981100	-1.97525200	2.32189800
C	-0.54620100	-1.75963200	3.02166200
C	0.47055700	-2.57384400	2.38264600
C	1.76348800	-2.08977800	2.24734900
C	2.49214400	-2.30202200	1.00982400
C	3.27771400	-1.11157600	0.74220500
C	3.43206500	-0.66049400	-0.56093200
C	0.22541500	0.49629500	-3.49621000
C	2.20157100	2.77187500	-0.03063800
C	1.55680600	2.92319000	-1.24976900
C	0.15379900	3.29309200	-1.28724100
C	-0.54238100	3.49590300	-0.10440700
C	0.13197200	3.33737900	1.17059400
C	1.94006000	2.00811200	2.17463900
C	2.95707700	1.19350800	1.53594200
C	3.11851600	1.66521200	0.17268700
C	3.35035000	0.75909000	-0.85180200
C	2.67655500	0.91756600	-2.12755400
C	1.79979000	1.97523300	-2.32187300
C	-0.47059700	2.57419500	-2.38264000
C	-1.76366900	2.09006100	-2.24731100
C	-2.49212100	2.30213000	-1.00985200
C	-1.89529500	2.98908600	0.03740200
C	-2.05710100	2.51761400	1.40061600
C	-0.80390900	2.73291900	2.10071000
C	-0.35697700	1.80059000	3.02592200

C	1.04586700	1.43012600	3.06374400
C	3.03540500	-0.16336000	1.81428400
C	2.09969200	-0.76843000	2.74444900
C	1.12716500	0.01042900	3.35427700
C	-0.22526300	-0.49637400	3.49602500
C	-1.14236500	0.60995600	3.29321300
C	-2.33976500	0.40425400	2.62439800
C	-2.80796400	1.37943300	1.65671800
C	-3.43210900	0.66046900	0.56090000
C	-3.27778800	1.11151300	-0.74213000
C	0.54646700	1.75975800	-3.02181300
C	-2.10001500	0.76834200	-2.74454100
C	1.47305500	2.98359200	1.20677200

C_{60}^{AB}

0 1

C	-1.44383300	0.34072800	-3.33832300
C	-2.67333900	0.52958500	-2.59057300
C	-2.85079600	1.67269300	-1.82531700
C	-1.80700300	2.68052900	-1.77163000
C	-0.63145400	2.49942100	-2.48549000
C	-0.44622700	1.30323900	-3.28686900
C	-1.09806900	-1.06740600	-3.28497300
C	-2.11365700	-1.74887500	-2.50256500
C	-3.08778500	-0.76181500	-2.07389800
C	-3.65989200	-0.85343200	-0.81303400
C	-3.44953300	1.57708200	-0.50667700
C	-1.75994800	3.20619300	-0.41993600
C	-0.54034000	3.52906100	0.15725700
C	0.68972500	3.34082900	-0.59028800
C	0.64456100	2.83741000	-1.88218000
C	1.61864500	1.85094900	-2.31077200
C	0.94416500	0.90259700	-3.17933500
C	1.27531700	-0.44364800	-3.12950500
C	0.23141400	-1.45091400	-3.18206800
C	-1.75492700	-2.78434600	-1.65177200
C	-0.36384200	-3.18510300	-1.54285400
C	0.60641500	-2.53394300	-2.29125700
C	1.88126100	-2.19505600	-1.68571900
C	2.29436800	-0.90310000	-2.20315200
C	2.93852500	0.00343500	-1.37500300
C	2.59482100	1.41243800	-1.42844200
C	2.64299200	1.93883600	-0.07721000
C	1.71123100	2.88057600	0.33280800
C	-2.77508300	2.52484200	0.36176900
C	0.45452300	1.06831500	3.28420100
C	-0.87489000	1.45174300	3.18138500
C	-1.91867000	0.44370700	3.12728700
C	-1.58803300	-0.90271100	3.18035000
C	-0.19719700	-1.30335900	3.28699300
C	2.02816100	-0.52882300	2.58866700
C	2.44425700	0.76322700	2.07322000
C	1.47064600	1.75004800	2.50338000

C	1.11157000	2.78439100	1.65175700
C	-0.27933000	3.18480500	1.54306200
C	-1.25035600	2.53440100	2.29116900
C	-2.93873800	0.90435600	2.20316100
C	-3.58352800	-0.00148400	1.37363200
C	-3.23699000	-1.41012300	1.42867200
C	-2.26128500	-1.85020100	2.31136000
C	-1.28738200	-2.83694100	1.88209800
C	-0.01179200	-2.49979700	2.48654600
C	1.16415300	-2.68149400	1.77271400
C	2.20808600	-1.67490700	1.82842500
C	3.01589500	0.85675100	0.81374100
C	3.19528200	-0.34005900	0.01251200
C	2.80520100	-1.57814400	0.50776100
C	2.13111400	-2.52708200	-0.36191900
C	1.11681200	-3.20743600	0.42057600
C	-0.10294900	-3.52997700	-0.15731600
C	-1.33263900	-3.34135000	0.59048900
C	-2.35350100	-2.88059000	-0.33311600
C	-3.28338100	-1.93654300	0.07696800
C	-2.52614800	2.19599800	1.68635400
C	-3.84474700	0.34253600	-0.01202700
C	0.79983700	-0.34029900	3.33765700
N	6.45122400	-0.73015400	0.00928700
H	6.77672800	-1.10138600	-0.88236400
H	7.07742400	-1.07105900	0.73748400
H	5.52013700	-1.11234000	0.18736600
B	6.41758500	0.92407400	-0.01341100
H	5.65431800	1.20839500	-0.91110000
H	6.01467200	1.24170700	1.08294900
H	7.56010200	1.25479500	-0.22881500

$C_{60}^{6-5}ts$

0 1			
C	-0.92946200	2.28455000	-2.36849000
C	0.19997500	3.01217300	-1.82253600
C	1.49240300	2.58674900	-2.09103300
C	1.71216400	1.41175900	-2.91837300
C	0.63248000	0.72343200	-3.45180300
C	-0.71924700	1.17159600	-3.17378400
C	-1.98990800	2.28896100	-1.38747900
C	-1.51437900	3.04643000	-0.21954100
C	-0.16015600	3.47086000	-0.49304300
C	0.80044200	3.48380800	0.51454700
C	2.49079600	2.58959300	-1.03770100
C	2.84008800	0.68422900	-2.37091900
C	2.83428900	-0.70591800	-2.37119800
C	1.70427700	-1.42693000	-2.92510200
C	0.62743400	-0.72859500	-3.45377200
C	-0.72721500	-1.16852000	-3.18176800
C	-1.55291000	0.00891800	-3.00103400
C	-2.56443200	0.02059700	-2.03902400
C	-2.80919700	1.19291000	-1.24232700

C	-1.85121000	2.59032700	1.03938500
C	-2.72771000	1.44537800	1.23378800
C	-3.40994700	0.79401000	0.09612600
C	-3.31767300	-0.74148200	0.10102500
C	-2.79016900	-1.14743800	-1.22127300
C	-2.00771500	-2.27064500	-1.39666300
C	-0.94667400	-2.27966200	-2.38305100
C	0.17772400	-3.01671500	-1.83482600
C	1.47375700	-2.59881700	-2.09927100
C	3.31629400	1.40609400	-1.20697400
C	2.59850900	-2.31046000	1.40013000
C	3.39822900	-1.18982600	1.23764000
C	3.17494000	-0.01406800	2.05953400
C	2.15746600	-0.00944700	3.00154300
C	1.31455700	-1.18178000	3.16847100
C	0.40923500	-3.03048300	1.84337000
C	0.76639700	-3.47347100	0.50911900
C	2.12300400	-3.03500300	0.23403700
C	2.46622600	-2.60470800	-1.03875700
C	3.30769200	-1.43312400	-1.21026400
C	3.75978400	-0.74017100	-0.09557900
C	3.40812400	1.16057300	1.23750200
C	2.62102000	2.29001400	1.39967600
C	1.55898800	2.29832900	2.38974500
C	1.33093200	1.17098100	3.16911200
C	-0.02511400	0.72923300	3.42536800
C	-0.03304400	-0.73421600	3.43964500
C	-1.11625400	-1.41631900	2.91408200
C	-0.88542300	-2.59376300	2.10094100
C	-0.18293600	-3.46572800	-0.50390800
C	-1.52753400	-2.99885500	-0.22645000
C	-1.86926100	-2.57751800	1.04334100
C	-2.69842200	-1.38672400	1.22005600
C	-2.27172200	-0.70264200	2.37510400
C	-2.23878300	0.71836000	2.31958000
C	-1.08956700	1.43151100	2.89965200
C	-0.85809300	2.60383100	2.09618700
C	0.43882600	3.03434200	1.83979500
C	3.76905800	0.70930500	-0.09514100
C	2.14714500	3.01980800	0.23508100
C	1.53886200	-2.31443900	2.39375400
N	-5.96581400	-0.70305500	0.01091700
H	-4.76044400	-0.96074800	0.10030800
H	-6.39067700	-1.11213600	0.84159200
H	-6.27211500	-1.21506100	-0.81491600
B	-6.06080700	0.80049500	-0.08942400
H	-6.41381500	1.37164900	0.89452800
H	-4.58172000	1.10779400	0.08219700
H	-6.17824200	1.24024400	-1.19052200

$C_{60}^{6-6}ts$

0 1

C	-0.25931500	3.47440500	0.69295100
---	-------------	------------	------------

C	0.90846300	3.00519000	1.42013200
C	2.01962100	2.54292300	0.72561300
C	2.01960200	2.54295100	-0.72555100
C	0.90843400	3.00524500	-1.42003600
C	-0.25933000	3.47443700	-0.69281800
C	-1.43761300	3.04277300	1.42001000
C	-0.99693300	2.30918900	2.59298300
C	0.45365000	2.28889300	2.58832300
C	1.13438100	1.15205500	3.00651200
C	2.74872400	1.38643500	1.18087500
C	2.74867700	1.38647500	-1.18086900
C	2.30044900	0.69218900	-2.28205300
C	1.13432700	1.15217200	-3.00649400
C	0.45360300	2.28899500	-2.58824900
C	-0.99698000	2.30929100	-2.59288100
C	-1.43764000	3.04283000	-1.41987300
C	-2.56608700	2.62830700	-0.72570400
C	-2.56607300	2.62827900	0.72584600
C	-1.70310000	1.19277000	3.01765000
C	-2.88373400	0.76179200	2.29531800
C	-3.30515300	1.46236000	1.17351200
C	-3.76457600	0.74293200	0.00004500
C	-3.30517400	1.46240600	-1.17340200
C	-2.88377500	0.76188100	-2.29524400
C	-1.70315400	1.19288700	-3.01757900
C	-0.99106800	0.00759200	-3.46313000
C	0.39637000	-0.01117100	-3.45493300
C	3.37008900	0.69047000	-0.00002100
C	0.82352300	-3.03681100	-1.42409000
C	1.94515000	-2.60926000	-0.72220400
C	1.94515700	-2.60928600	0.72205700
C	0.82354500	-3.03686400	1.42395000
C	-0.35343800	-3.47275800	0.69380100
C	-1.52024100	-3.00891400	-1.42093800
C	-1.05779800	-2.28816900	-2.59516300
C	0.39217300	-2.31673800	-2.59894300
C	1.11074800	-1.19668900	-3.01090600
C	2.29647600	-0.77502100	-2.30445500
C	2.69167700	-1.44951300	-1.16209400
C	2.69166900	-1.44954500	1.16197300
C	2.29651700	-0.77510800	2.30438400
C	1.11080000	-1.19680400	3.01083400
C	0.39221800	-2.31683900	2.59884100
C	-1.05775200	-2.28827000	2.59508700
C	-1.52021600	-3.00896900	1.42084400
C	-2.63491600	-2.56263300	0.72613000
C	-2.63492800	-2.56260500	-0.72618700
C	-1.73743700	-1.15663700	-3.02359700
C	-2.90222000	-0.69067800	-2.29530200
C	-3.34403700	-1.37824600	-1.17401800
C	-3.77980500	-0.64482800	0.00001900
C	-3.34401600	-1.37829200	1.17402000
C	-2.90217900	-0.69076700	2.29532300
C	-1.73738400	-1.15675400	3.02357900
C	-0.99100600	0.00745800	3.46314300

C	0.39643100	-0.01130400	3.45492100
C	3.27108300	-0.77628500	-0.00004300
C	2.30049000	0.69209900	2.28203000
C	-0.35344800	-3.47272800	-0.69393400
N	6.00070800	-0.68851200	0.00002500
H	6.42136400	-1.10671600	0.82896800
H	6.42118900	-1.10676900	-0.82898000
H	4.92617000	-1.00244000	0.00013500
B	6.00975900	0.85818800	-0.00002400
H	4.62739500	1.06777700	-0.00009900
H	6.31444700	1.34083900	1.04781900
H	6.31455500	1.34078100	-1.04786300

C_{60}^{6-6}

0 1

C	-0.04279000	3.47871500	0.69329300
C	1.12960800	3.02534600	1.42193100
C	2.24670900	2.57371400	0.72521100
C	2.24673200	2.57380400	-0.72494700
C	1.12965400	3.02551800	-1.42163000
C	-0.04276400	3.47878600	-0.69295000
C	-1.21473300	3.03036000	1.42054300
C	-0.76163600	2.30252700	2.59286600
C	0.68850300	2.30619600	2.58829100
C	1.38980200	1.17448000	2.99433800
C	2.99369500	1.43200900	1.17429400
C	2.99382400	1.43215900	-1.17411200
C	2.56386300	0.74115000	-2.27608200
C	1.38987200	1.17476200	-2.99414500
C	0.68856200	2.30644800	-2.58806200
C	-0.76158500	2.30277800	-2.59266700
C	-1.21469300	3.03050600	-1.42027700
C	-2.33638100	2.59822400	-0.72588500
C	-2.33641600	2.59815000	0.72609700
C	-1.45212600	1.17574600	3.01724600
C	-2.62448700	0.72731300	2.29444900
C	-3.05800700	1.42200900	1.17348500
C	-3.50493900	0.69467300	0.00000000
C	-3.05797300	1.42213600	-1.17339900
C	-2.62444500	0.72752100	-2.29441000
C	-1.45207000	1.17601400	-3.01712000
C	-0.72170600	0.00034700	-3.45714000
C	0.66504100	0.00003400	-3.43882400
C	3.73257300	0.78981500	0.00008300
C	1.12825500	-3.02578600	-1.42190800
C	2.24556800	-2.57463200	-0.72514700
C	2.24557400	-2.57472700	0.72499500
C	1.12824900	-3.02596700	1.42166300
C	-0.04435900	-3.47873400	0.69293800
C	-1.21609100	-3.02987100	-1.42056200
C	-0.76266400	-2.30217100	-2.59287100
C	0.68746700	-2.30649000	-2.58825200
C	1.38932300	-1.17511400	-2.99430800

C	2.56355000	-0.74210100	-2.27627300
C	2.99312000	-1.43337000	-1.17428700
C	2.99325700	-1.43353400	1.17423700
C	2.56348500	-0.74229100	2.27616800
C	1.38926200	-1.17539400	2.99416400
C	0.68742200	-2.30675200	2.58806000
C	-0.76272300	-2.30242500	2.59265100
C	-1.21610400	-3.03000600	1.42024400
C	-2.33756600	-2.59726600	0.72583200
C	-2.33757000	-2.59718300	-0.72614500
C	-1.45260800	-1.17507900	-3.01725000
C	-2.62479200	-0.72615100	-2.29447200
C	-3.05861800	-1.42066800	-1.17352000
C	-3.50526700	-0.69315900	-0.00006600
C	-3.05863700	-1.42080500	1.17331800
C	-2.62483000	-0.72635900	2.29432300
C	-1.45268000	-1.17534800	3.01706900
C	-0.72178100	-0.00001800	3.45712600
C	0.66496700	-0.00034400	3.43883300
C	3.73244200	-0.79141600	-0.00003000
C	2.56381500	0.74094100	2.27627600
C	-0.04436300	-3.47869300	-0.69328600
H	4.77943700	-1.11572500	-0.00020900
H	4.77983300	1.11374500	0.00024100

C_{60}^{6-5}

0 1

C	-1.18741500	2.31119900	-2.43891400
C	-0.09016800	3.04458500	-1.84918500
C	1.21850200	2.61451400	-2.05187100
C	1.47890600	1.43417400	-2.83394100
C	0.43482000	0.73559900	-3.39394300
C	-0.92590400	1.17662300	-3.20143100
C	-2.28971200	2.30333500	-1.49330400
C	-1.86365000	3.03316900	-0.31049100
C	-0.50205800	3.48784200	-0.53569800
C	0.41487800	3.47180300	0.50979100
C	2.16897100	2.60384400	-0.96143700
C	2.61198600	0.72459600	-2.20586700
C	2.61203700	-0.72731000	-2.20480900
C	1.47903300	-1.43781000	-2.83199900
C	0.43489300	-0.74007600	-3.39297900
C	-0.92581000	-1.18094300	-3.19990900
C	-1.76411300	-0.00210300	-3.06937500
C	-2.82102400	-0.00153500	-2.17287400
C	-3.08383600	1.17495700	-1.36239400
C	-2.25389200	2.59955900	0.94647400
C	-3.09206300	1.42016300	1.08479400
C	-3.49935900	0.72401000	-0.04547500
C	-3.49929700	-0.72432200	-0.04453300
C	-3.08373700	-1.17696300	-1.36086200
C	-2.28951500	-2.30544600	-1.49029700
C	-1.18723400	-2.31451300	-2.43589600

C	-0.08993100	-3.04707800	-1.84523600
C	1.21869200	-2.61712900	-2.04842200
C	3.03507600	1.42671300	-1.11131400
C	2.20814500	-2.27015100	1.48099300
C	3.01946300	-1.16755800	1.35552200
C	2.73646700	0.00150900	2.13362200
C	1.68874600	0.00209100	3.06591600
C	0.85896500	-1.16447400	3.21298600
C	0.00376500	-3.00997500	1.82571400
C	0.41514600	-3.47108800	0.51429200
C	1.77592800	-3.02853300	0.28952500
C	2.16922300	-2.60489000	-0.95803500
C	3.03516800	-1.42792800	-1.10940500
C	3.75633800	-0.80242300	0.06319700
C	3.01935800	1.16958900	1.35405000
C	2.20796300	2.27228600	1.47810200
C	1.10821800	2.27576400	2.40973900
C	0.85885500	1.16877200	3.21148100
C	-0.50423500	0.72839700	3.43558600
C	-0.50415900	-0.72391700	3.43649700
C	-1.55927400	-1.41812800	2.86234200
C	-1.29981400	-2.59177200	2.04442300
C	-0.50180700	-3.48863500	-0.53115400
C	-1.86342600	-3.03373100	-0.30653700
C	-2.25368200	-2.59847400	0.94985500
C	-3.09195300	-1.41895700	1.08663700
C	-2.66300100	-0.69488100	2.26526700
C	-2.66306100	0.69766300	2.26437100
C	-1.55941400	1.42177700	2.86053400
C	-1.30002300	2.59435500	2.04105300
C	0.00351500	3.01241300	1.82182500
C	3.75625700	0.80277400	0.06211700
C	1.77569700	3.02904900	0.28559100
C	1.10840300	-2.27246100	2.41265900
H	4.79739500	1.14344700	0.09707700
H	4.79750400	-1.14298200	0.09869700

C₇₀

0 1

C	-3.21870800	-2.34554900	-0.52936100
C	-2.43928000	-2.44761000	-1.74247900
C	-3.96589900	-1.20308000	-0.27163800
C	-2.43903400	-1.41077900	-2.65211700
C	-1.20108800	-1.02045800	-3.30196400
C	-0.00002000	-1.73987700	-3.09647800
C	1.20097500	-1.02034600	-3.30220600
C	-3.21882800	-1.22838000	2.06701400
C	-2.43893000	-2.41353200	1.78937900
C	-3.96599400	-0.63039800	1.05986800
C	-2.43894700	-2.95829700	0.52227300
C	-1.20082700	-3.45566100	-0.04942900
C	0.00006400	-3.48345100	0.69877400
C	1.20081800	-3.45603200	-0.04953500
C	0.00004200	-2.84394900	-2.12690700

C	-1.20079600	-3.14125700	-1.44003100
C	1.20076500	-3.14162300	-1.44004600
C	-3.21924400	1.58624200	1.80707500
C	-2.43900600	0.95602200	2.84810300
C	-3.96649700	0.81346100	0.92697000
C	-2.43878300	-0.41720300	2.97451500
C	-1.20072300	-1.11472500	3.27090700
C	0.00007200	-0.41176700	3.52788300
C	1.20089100	-1.11483300	3.27099700
C	0.00008000	-2.90193000	2.04808900
C	-1.20071500	-2.34024800	2.54276100
C	1.20092500	-2.34029600	2.54289800
C	-3.21864800	2.20841500	-0.94997200
C	-2.43892500	3.00373100	-0.02862000
C	-3.96621800	1.13287800	-0.48727600
C	-2.43893100	2.70000100	1.31641100
C	-1.20081400	2.76645700	2.07127100
C	0.00009700	3.22847800	1.48227500
C	1.20100600	2.76651400	2.07132300
C	0.00007700	1.05076500	3.39202600
C	-1.20063400	1.69512000	3.01104600
C	1.20078000	1.69520100	3.01111700
C	-3.21883900	-0.22122000	-2.39400200
C	-2.43902500	0.90128400	-2.86558900
C	-3.96631000	-0.11373700	-1.22797900
C	-2.43862900	2.08649700	-2.16091500
C	-1.20073000	2.82505100	-1.99067600
C	-0.00001300	2.40702200	-2.61213800
C	1.20070000	2.82509800	-1.99078600
C	0.00002700	3.55203000	0.04916100
C	-1.20075800	3.38798400	-0.68132000
C	1.20075400	3.38800300	-0.68145700
C	-0.00006400	1.14400300	-3.36270800
C	-1.20105400	0.39888400	-3.43291200
C	1.20094600	0.39892600	-3.43308200
C	3.21865700	2.20837900	-0.94998400
C	2.43862800	2.08648500	-2.16093100
C	2.43886600	0.90127600	-2.86568200
C	3.96627600	1.13275800	-0.48743100
C	3.21928500	1.58621600	1.80690300
C	2.43899400	2.70000400	1.31631100
C	2.43890000	3.00376400	-0.02872100
C	3.96661200	0.81340000	0.92680800
C	3.21874900	-1.22838600	2.06673500
C	2.43887800	-0.41729900	2.97444000
C	2.43910400	0.95598100	2.84791700
C	3.96620400	-0.63034500	1.05988500
C	3.21850700	-2.34545400	-0.52946900
C	2.43868400	-2.95834400	0.52225400
C	2.43904400	-2.41360600	1.78926600
C	3.96594300	-1.20309800	-0.27176300
C	3.21851300	-0.22130300	-2.39405200
C	2.43874700	-1.41081500	-2.65210400
C	2.43901600	-2.44773500	-1.74264400
C	3.96628600	-0.11371000	-1.22825400

C_{70}^{AB}

0 1

C	-3.68568600	-0.46952900	-0.25496300
C	-3.11934800	-1.05110100	-1.45203100
C	-3.78758900	0.91188900	-0.12466900
C	-2.67818100	-0.23353000	-2.47057600
C	-1.44243800	-0.54732200	-3.16450800
C	-0.71925200	-1.73022600	-2.88137500
C	0.66558300	-1.69641600	-3.16967300
C	-3.01287300	0.75691900	2.19813600
C	-2.90893300	-0.67850500	2.05391400
C	-3.44335900	1.54215000	1.13616500
C	-3.23604900	-1.27806500	0.85719400
C	-2.41955600	-2.35988000	0.34049000
C	-1.33635700	-2.88390100	1.08365700
C	-0.31028600	-3.50612500	0.33415000
C	-1.19031300	-2.60022100	-1.79520700
C	-2.34761400	-2.22044600	-1.07531400
C	-0.23874300	-3.36695900	-1.08243800
C	-1.69058500	3.18834500	1.62744000
C	-1.24801400	2.36579600	2.73036400
C	-2.76410000	2.78763300	0.84127600
C	-1.89335900	1.17899400	3.00968500
C	-1.12166400	0.00681400	3.37856300
C	0.28164100	0.07141600	3.55200700
C	0.98735100	-1.14136400	3.37213600
C	-0.98505500	-2.24590300	2.36052100
C	-1.74465300	-1.13276900	2.79252000
C	0.36410200	-2.28118800	2.78546200
C	-1.54906500	3.46559400	-1.18179500
C	-0.43459700	3.87546200	-0.35738300
C	-2.69150500	2.92918800	-0.60000900
C	-0.50404600	3.74019300	1.01344700
C	0.65647700	3.27938800	1.75322900
C	1.89724500	3.05034800	1.11231100
C	2.76527800	2.13008500	1.74595200
C	0.96952900	1.33515300	3.25399800
C	0.20011000	2.43558600	2.80752000
C	2.30874600	1.28577400	2.79988400
C	-2.78238900	1.20373800	-2.34464300
C	-1.59168700	1.76470400	-2.94154700
C	-3.32449600	1.77094700	-1.19819300
C	-0.98962900	2.86838600	-2.37358700
C	0.45805000	2.93632500	-2.29055300
C	1.27888800	1.93630000	-2.86378400
C	2.56665200	1.78640300	-2.29638300
C	1.97175700	3.19423600	-0.34786700
C	0.79859500	3.55486700	-1.05297400
C	2.90766400	2.40559700	-1.05868900
C	0.63700000	0.76152800	-3.46941700
C	-0.77558400	0.67857100	-3.45273200
C	1.33283000	-0.47030100	-3.45899300

C	4.10342700	0.38418000	-1.19942200
C	3.29349300	0.53350300	-2.38723500
C	2.69042500	-0.56952500	-2.95472400
C	4.27419800	-0.86757900	-0.62092600
C	3.96098700	0.10820300	1.60986200
C	3.77857400	1.40620700	1.00019300
C	3.84852500	1.54093200	-0.37047700
C	4.20144100	-1.00903100	0.81991800
C	2.63836700	-2.32280100	2.18256400
C	2.38905100	-1.15394300	2.99612000
C	3.03517000	0.03202900	2.71706000
C	3.52321400	-2.25640100	1.11385100
C	1.96243800	-3.54895600	-0.27202400
C	1.04492200	-3.60872500	0.84344000
C	1.37464800	-3.01096400	2.04161000
C	3.17655800	-2.88574300	-0.14570100
C	2.86815500	-1.87588200	-2.36203900
C	1.60387800	-2.56643000	-2.48446800
C	1.16156700	-3.38178800	-1.46408700
C	3.64087800	-2.02703800	-1.21764900
N	-6.84897300	-1.41694300	-0.08143300
H	-7.33503300	-1.33544200	-0.97352200
H	-7.52346400	-1.23525400	0.66059600
H	-6.13362200	-0.68799100	-0.04745500
B	-6.16941600	-2.91604900	0.08497700
H	-5.37794100	-3.00085200	-0.82893800
H	-5.64739500	-2.90218000	1.17728000
H	-7.09511900	-3.68841800	-0.00234400

$C_{70}^{6-5}ts$

0 1

C	2.52860900	1.92087900	2.27495000
C	1.28011800	2.03883100	2.98997600
C	2.78669500	2.72625000	1.17215600
C	0.33247200	2.94752200	2.57510900
C	-1.07360900	2.57873600	2.57635100
C	-1.51140300	1.33326100	3.08883000
C	-2.73795600	0.84622100	2.57696700
C	3.71651100	0.78625100	0.00001500
C	3.48322300	-0.02845100	1.16004100
C	3.38958900	2.14177900	-0.00003500
C	2.87568100	0.52088000	2.25882800
C	1.84479000	-0.21445800	2.99346200
C	1.48237800	-1.53022000	2.61034900
C	0.18456200	-1.94486900	2.98728200
C	-0.50357400	0.36469000	3.53836800
C	0.87282500	0.71321900	3.43073300
C	-0.79868000	-1.00743100	3.44247100
C	2.51613700	1.94735800	-2.27678800
C	2.86390300	0.54713100	-2.27500500
C	2.78059700	2.74493400	-1.17084100
C	3.43130400	-0.02478900	-1.15871400
C	3.15832600	-1.40330200	-0.76180400

C	2.10303900	-2.11155800	-1.45141300
C	1.40778100	-3.10493600	-0.75275700
C	2.11111700	-2.13779000	1.44468600
C	3.24839700	-1.46191400	0.75138900
C	1.39281900	-3.06767400	0.70979700
C	0.57977600	3.80535700	-1.40260600
C	0.31628500	2.98239700	-2.55767800
C	1.78715400	3.69227100	-0.71852600
C	1.26145000	2.07049300	-2.98448700
C	0.85132700	0.75563000	-3.43539300
C	-0.51900300	0.39758100	-3.52955000
C	-0.81391300	-0.97899000	-3.44978300
C	1.46968000	-1.50285100	-2.62545300
C	1.82197000	-0.17762700	-2.98172000
C	0.16943200	-1.91832600	-2.99626600
C	0.58932000	3.78611900	1.42310200
C	-0.65911500	3.90244700	0.70645400
C	1.78944200	3.68352800	0.73244000
C	-0.66403500	3.90955600	-0.67270600
C	-1.69033000	3.17881500	-1.39457000
C	-2.75078800	2.52805600	-0.71793900
C	-3.35461000	1.44494100	-1.39800500
C	-1.52692300	1.36241100	-3.06949500
C	-1.08721800	2.60434300	-2.54888600
C	-2.74916800	0.86819500	-2.55435500
C	-2.74590700	2.52027300	0.75128400
C	-1.67895500	3.16120500	1.42864200
C	-3.34392600	1.43007400	1.42411000
C	-3.86727100	-0.85245800	-1.41124000
C	-4.03590500	0.38478800	-0.67988300
C	-4.03440000	0.37858500	0.69949300
C	-3.69114500	-2.05111600	-0.72821700
C	-1.91885000	-2.70261000	-2.29572300
C	-2.10489400	-1.45130600	-2.99939000
C	-3.05854800	-0.54906500	-2.56657700
C	-2.69745700	-2.99951700	-1.18295900
C	-0.70503800	-3.84188900	-0.01560900
C	0.10087300	-3.53473600	-1.17971000
C	-0.50312500	-2.98620300	-2.30050500
C	-2.06983800	-3.58261300	-0.01207500
C	-1.91622900	-2.72097700	2.28462500
C	-0.49579600	-2.99226300	2.27158000
C	0.09409000	-3.53509800	1.14611700
C	-2.68851200	-3.00560600	1.16653200
C	-3.86118600	-0.86435900	1.41658700
C	-3.04657300	-0.57014200	2.57517700
C	-2.09809600	-1.47807200	2.99998500
C	-3.68862400	-2.05522500	0.72259800
N	5.37997500	-2.90870200	-0.70770600
H	4.45656900	-2.26007400	-0.98324100
H	6.17569600	-2.47502800	-1.17415300
H	5.20233500	-3.82115600	-1.12698300
B	5.45793200	-2.91539800	0.81761700
H	6.28046500	-2.19146200	1.28585500
H	4.26786100	-2.09680500	1.07972400

H 5.08117300 -3.91696400 1.34173500

$C_{70}^{6-6}ts$

0 1

C	3.03057000	0.32672400	-2.29048900
C	2.63952800	-1.07905300	-2.26177600
C	3.60897600	0.87880100	-1.15885300
C	2.89171400	-1.86115400	-1.16840100
C	1.88476900	-2.78794300	-0.71212300
C	0.69613500	-3.02722900	-1.44493900
C	-0.40671200	-3.52656400	-0.71160600
C	2.20318400	2.88471700	-1.41812300
C	1.58548000	2.29328800	-2.57003600
C	3.19279000	2.19106500	-0.71993200
C	1.98262400	1.03138000	-2.97963200
C	0.98303900	0.07359200	-3.41758400
C	-0.38544500	0.42031400	-3.52219800
C	-1.30820900	-0.64889700	-3.43219400
C	0.43774800	-2.20834400	-2.62949100
C	1.38607000	-1.21905300	-2.97765500
C	-0.90422400	-1.94256900	-2.99320100
C	2.20311600	2.88514000	1.41740400
C	1.16831300	3.58548400	0.68940700
C	3.19275800	2.19127800	0.71947200
C	1.16834600	3.58527800	-0.69038700
C	-0.08241300	3.43783600	-1.41210500
C	-1.32422900	3.38058700	-0.73577800
C	-2.37287700	2.71399300	-1.41187300
C	-0.80737500	1.75498700	-3.07483200
C	0.17355000	2.63628700	-2.56332400
C	-2.11693700	1.91178700	-2.56093200
C	3.03045300	0.32740700	2.29057200
C	1.98247300	1.03226900	2.97945100
C	3.60892800	0.87914100	1.15880500
C	1.58534900	2.29405300	2.56945800
C	0.17342100	2.63705000	2.56257500
C	-0.80753100	1.75590300	3.07429500
C	-2.11706800	1.91255000	2.56028200
C	-1.32426600	3.38080600	0.73473200
C	-0.08248400	3.43825700	1.41110600
C	-2.37294900	2.71441400	1.41097200
C	3.68479400	-1.35979700	0.00030700
C	2.89163900	-1.86079800	1.16912600
C	4.00009200	0.07468800	0.00010100
C	2.63941100	-1.07837500	2.26226100
C	1.38591700	-1.21816400	2.97812000
C	0.43761600	-2.20756000	2.63019700
C	-0.90437500	-1.94167400	2.99375400
C	-0.38562400	0.42136300	3.52207800
C	0.98286500	0.07461200	3.41763900
C	-1.30838300	-0.64787400	3.43234500
C	0.69606200	-3.02680200	1.44590400
C	1.88473000	-2.78773500	0.71306900

C	-0.40674900	-3.52635900	0.71266700
C	-3.12290000	-1.61402200	2.28631300
C	-2.01353100	-2.54158600	2.27702400
C	-1.76978400	-3.31726400	1.16202700
C	-3.94502100	-1.49420300	1.17290400
C	-3.93094100	0.94943300	1.41154800
C	-3.06948600	0.81614400	2.56409600
C	-2.67561700	-0.43420400	2.99250700
C	-4.36092700	-0.18039500	0.72427200
C	-3.93086900	0.94901200	-1.41200500
C	-3.48405200	2.11792800	-0.68963300
C	-3.48408700	2.11813300	0.68885200
C	-4.36089000	-0.18061100	-0.72441400
C	-3.12278500	-1.61470300	-2.28596700
C	-2.67546500	-0.43509500	-2.99248900
C	-3.06935600	0.81538000	-2.56446900
C	-3.94496200	-1.49455300	-1.17263500
C	-2.62414800	-3.20138500	0.00042300
C	-1.76972200	-3.31760000	-1.16110000
C	-2.01341600	-2.54226500	-2.27634700
C	-3.68721600	-2.30844400	0.00026300
N	6.59215900	-0.77206700	0.00047400
H	7.11119700	-0.48378300	-0.82803800
H	7.11099000	-0.48486700	0.82949500
H	5.64347900	-0.17315700	0.00071600
B	6.17659900	-2.26106800	-0.00051100
H	4.79089400	-2.08361000	0.00046600
H	6.33861100	-2.80785400	-1.04872900
H	6.34008400	-2.80975800	1.04648300

C_{70}^{6-5}

0 1

C	-3.15190400	-2.25757000	0.86726100
C	-2.40476600	-2.99463300	-0.16329900
C	-3.92248700	-1.16466900	0.53917100
C	-2.46300000	-2.57758100	-1.46227500
C	-1.25145000	-2.58480100	-2.26041300
C	-0.02579100	-3.10266700	-1.76916900
C	1.14557600	-2.57832900	-2.35436700
C	-3.07321600	-0.00116900	2.53082100
C	-2.29285900	-1.15355000	2.87375600
C	-3.86538400	-0.00060200	1.36709400
C	-2.32013300	-2.25030000	2.03541300
C	-1.09435900	-2.98053800	1.75300200
C	0.12922800	-2.63299200	2.37448400
C	1.30378800	-2.99770500	1.67499800
C	0.03010300	-3.55086200	-0.37521200
C	-1.14731200	-3.43750100	0.40793600
C	1.25513800	-3.44783100	0.32227000
C	-3.15171200	2.25679900	0.86929300
C	-2.32000600	2.24838700	2.03746600
C	-3.92239000	1.16424300	0.54022000
C	-2.29278900	1.15091300	2.87480800

C	-1.03156800	0.71056300	3.44152000
C	0.16236000	1.44532800	3.24695900
C	1.36732100	0.71184400	3.33781500
C	0.16229200	-1.44846300	3.24555100
C	-1.03159800	-0.71380900	3.44087100
C	1.36727100	-0.71511700	3.33708400
C	-3.27325300	1.42404000	-1.83183000
C	-2.46293900	2.57898500	-1.45982900
C	-4.28933000	0.80333000	-0.90197400
C	-2.40454900	2.99482400	-0.16047600
C	-1.14709800	3.43718700	0.41121000
C	0.03031400	3.55130400	-0.37177200
C	1.25532900	3.44747000	0.32568400
C	0.12936200	2.63066200	2.37702900
C	-1.09417700	2.97884400	1.75581500
C	1.30395300	2.99598400	1.67789300
C	-3.27333400	-1.42218500	-1.83326600
C	-2.55069600	-0.71818700	-2.75736700
C	-4.28953700	-0.80217600	-0.90279300
C	-2.55072300	0.72099800	-2.75646800
C	-1.29269900	1.42304600	-3.05753900
C	-0.11513600	0.74167600	-3.42737400
C	1.10014700	1.41503800	-3.17640500
C	-0.02559200	3.10448300	-1.76621800
C	-1.25127900	2.58709200	-2.25786600
C	1.14572000	2.58057500	-2.35186200
C	-0.11516400	-0.73827200	-3.42814300
C	-1.29272000	-1.41996100	-3.05903900
C	1.10008000	-1.41195900	-3.17777600
C	3.17057900	1.41463600	-2.06009500
C	2.34631800	0.69089500	-2.99988800
C	2.34631000	-0.68810400	-3.00056100
C	3.95798900	0.72530400	-1.14466700
C	3.28397200	2.28823900	0.62358200
C	2.47013000	3.00325800	-0.33517300
C	2.41472100	2.57483500	-1.64470700
C	4.01673600	1.17447000	0.23188000
C	3.34435100	-0.00119700	2.28040000
C	2.57870900	1.15995200	2.67618600
C	2.55130000	2.27766400	1.86864400
C	4.04592400	-0.00064000	1.08237900
C	3.28378700	-2.28897300	0.62135100
C	2.55114100	-2.27959600	1.86642100
C	2.57861100	-1.16267300	2.67506600
C	4.01664200	-1.17488200	0.23073900
C	3.17053300	-1.41281500	-2.06146000
C	2.41457800	-2.57333400	-1.64725300
C	2.46997500	-3.00306800	-0.33810200
C	3.95794700	-0.72439600	-1.14536400
H	-5.30189800	-1.14341200	-1.14679700
H	-5.30181100	1.14485200	-1.14560100

0 1

C	-3.23072800	-0.54983500	2.26145100
C	-2.50934000	-1.83403500	2.25678200
C	-3.96204300	-0.15108900	1.17055300
C	-2.55329100	-2.64204300	1.16218500
C	-1.34660900	-3.28088200	0.71068800
C	-0.13420000	-3.21999400	1.44562600
C	1.05605500	-3.42969800	0.71150800
C	-3.07686100	2.13431900	1.41731100
C	-2.32780100	1.71024900	2.55934500
C	-3.85756800	1.20647900	0.72327600
C	-2.39371600	0.38728200	2.96206500
C	-1.19342300	-0.29186300	3.40293600
C	0.04534400	0.38529800	3.51594000
C	1.20649300	-0.41842400	3.43255900
C	-0.09261200	-2.36678400	2.62883900
C	-1.26306300	-1.64621800	2.96797100
C	1.13872300	-1.77281700	2.99357500
C	-3.07686700	2.13573800	-1.41507500
C	-2.24813900	3.07294600	-0.68765200
C	-3.85751200	1.20719600	-0.72189000
C	-2.24810700	3.07214500	0.69075400
C	-1.00071000	3.24013100	1.41183100
C	0.21810200	3.49527100	0.73665700
C	1.39792600	3.10750600	1.41212200
C	0.12081900	1.78387300	3.07059700
C	-1.04791400	2.39656600	2.55935900
C	1.34970200	2.26449000	2.56073300
C	-3.23095800	-0.54753300	-2.26213800
C	-2.39386600	0.39028000	-2.96163200
C	-3.96186400	-0.14987800	-1.17052600
C	-2.32790000	1.71288100	-2.55761800
C	-1.04799800	2.39915600	-2.55693700
C	0.12074000	1.78702800	-3.06882200
C	1.34965800	2.26713900	-2.55851600
C	0.21809100	3.49602800	-0.73317700
C	-1.00073400	3.24153500	-1.40854500
C	1.39792500	3.10896300	-1.40904400
C	-3.51566100	-2.44555700	-0.00114600
C	-2.55342000	-2.64092500	-1.16478200
C	-4.30211800	-1.07336100	-0.00053000
C	-2.50939900	-1.83167000	-2.25844200
C	-1.26314200	-1.64315100	-2.96951400
C	-0.09267800	-2.36406500	-2.63118000
C	1.13862200	-1.76973800	-2.99535700
C	0.04523500	0.38888400	-3.51555300
C	-1.19354100	-0.28839200	-3.40321200
C	1.20638400	-0.41491700	-3.43301800
C	-0.13425700	-3.21854100	-1.44887000
C	-1.34663700	-3.28010200	-0.71398700
C	1.05602100	-3.42897900	-0.71497900
C	3.20396200	-0.89718100	-2.28704600
C	2.36210800	-2.07220000	-2.27737700
C	2.32317700	-2.88672700	-1.16355600
C	3.96942700	-0.57616300	-1.17285500

C	3.34614500	1.78640000	-1.41108100
C	2.54510300	1.44260500	-2.56272300
C	2.47552100	0.13384200	-2.99184300
C	4.04502100	0.79968000	-0.72342100
C	3.34617300	1.78494300	1.41281400
C	2.62271800	2.80626800	0.69083500
C	2.62271200	2.80699000	-0.68805600
C	4.04506000	0.79893700	0.72415100
C	3.20403400	-0.89952700	2.28606500
C	2.47559700	0.13078700	2.99191000
C	2.54518200	1.43998700	2.56412400
C	3.96946300	-0.57737400	1.17219000
C	3.12090700	-2.56035100	-0.00133700
C	2.32322500	-2.88790700	1.16059000
C	2.36218800	-2.07454100	2.27525400
C	3.92641700	-1.42904800	-0.00077900
H	-4.26053000	-3.25058600	-0.00140500
H	-5.37129600	-1.31129500	-0.00085200

C₃₆

0 1

C	0.72037100	0.98577600	2.26365900
C	1.41217200	-0.25911500	2.27902200
C	0.72039600	-1.46830400	1.98526000
C	1.41250400	-2.10393800	0.91537100
C	0.72065500	-2.45500100	-0.27873600
C	1.41286800	-1.84524700	-1.36377000
C	0.72037400	-0.98577400	-2.26365300
C	1.41217700	0.25911600	-2.27902600
C	0.72039700	1.46830400	-1.98525300
C	1.41250500	2.10394000	-0.91537100
C	0.72065400	2.45500100	0.27874100
C	1.41286300	1.84524500	1.36376800
C	-0.72041000	0.98574000	2.26358400
C	-1.41293400	1.84541900	1.36377900
C	-0.72068200	2.45490700	0.27872900
C	-1.41257300	2.10406500	-0.91553100
C	-0.72042900	1.46827300	-1.98520700
C	-1.41224600	0.25904800	-2.27920700
C	-0.72040700	-0.98573900	-2.26357600
C	-1.41293600	-1.84542200	-1.36378400
C	-0.72068100	-2.45490600	-0.27872200
C	-1.41257100	-2.10406500	0.91552900
C	-0.72042900	-1.46827400	1.98521500
C	-1.41224300	-0.25904800	2.27920100
C	-2.60680900	-0.15826400	1.39552800
C	-2.60676200	1.12947400	0.83461000
C	-2.60688100	1.28814100	-0.56097100
C	-2.60680800	0.15826200	-1.39553400
C	-2.60676000	-1.12947600	-0.83461600
C	-2.60688000	-1.28814100	0.56096700
C	2.60690900	-0.15831600	1.39550300

C	2.60698100	-1.28814500	0.56090300
C	2.60686300	-1.12942700	-0.83465100
C	2.60690900	0.15831800	-1.39550600
C	2.60698000	1.28814600	-0.56090400
C	2.60686300	1.12942700	0.83464900

C_{36}^{AB}

0 1

C	0.03357700	-0.65720100	-2.46456200
C	1.01866900	-1.62177400	-2.11689700
C	2.21326100	-1.21643600	-1.44925500
C	2.31676400	-1.96746900	-0.24319100
C	2.44325600	-1.30104800	1.00816000
C	1.39167100	-1.76006000	1.85865400
C	0.49516900	-0.82816200	2.44817200
C	-0.83711900	-1.20373500	2.08735300
C	-1.68419000	-0.26895100	1.43220900
C	-2.14872100	-0.85971000	0.21340300
C	-1.91264200	-0.18376100	-1.02522000
C	-1.20899600	-1.06629300	-1.88951800
C	0.38364200	0.74064400	-2.45031900
C	-0.50585200	1.67078000	-1.83451900
C	-1.56601300	1.21575400	-1.00848400
C	-1.42509100	1.88078100	0.24180300
C	-1.33624700	1.13081200	1.44750800
C	-0.13450900	1.53363000	2.09141100
C	0.84617200	0.56915100	2.46477500
C	2.06541200	0.98255700	1.86422000
C	2.79637700	0.09415900	1.02432400
C	2.97871800	0.77416500	-0.21165400
C	2.56559900	0.17967600	-1.43456000
C	1.69441900	1.11932800	-2.06029200
C	1.63695600	2.37358300	-1.25007100
C	0.28254300	2.71090300	-1.10990700
C	-0.28170600	2.83714900	0.16847100
C	0.51036800	2.62612300	1.30686100
C	1.86519200	2.28848700	1.16663900
C	2.42699500	2.16161900	-0.11121400
C	0.36781800	-2.68565000	-1.30908800
C	1.15932300	-2.89688400	-0.16659500
C	0.59490300	-2.76935900	1.11458100
C	-0.76322000	-2.42890100	1.25481400
C	-1.55651700	-2.21803800	0.11175000
C	-0.98950700	-2.34522600	-1.17021100
N	-5.38415700	-0.23900000	0.11461700
H	-5.99484300	-0.62220400	-0.60563900
H	-5.83357700	-0.38352500	1.01778500
H	-4.50888800	-0.76957900	0.10999700
B	-5.07301600	1.35918100	-0.14691600
H	-4.56386400	1.40366600	-1.24542200
H	-6.14740400	1.90996500	-0.08838200
H	-4.31610600	1.67493100	0.74661200

$C_{36}^{6-6}ts$

0 1

C	-0.88987300	-0.60100200	-2.12866000
C	0.22794900	-1.41967500	-2.31754200
C	1.58256700	-0.88633600	-2.13271400
C	2.22459800	-1.66852600	-1.16190300
C	2.81344100	-1.06140700	0.00040300
C	2.22422300	-1.66850100	1.16255000
C	1.58185900	-0.88626900	2.13310800
C	0.22719200	-1.41962200	2.31755400
C	-0.89056900	-0.60094500	2.12821500
C	-1.78490300	-1.22259300	1.15856200
C	-2.24831900	-0.48153800	-0.00043600
C	-1.78448400	-1.22261000	-1.15920500
C	-0.73170000	0.83237500	-2.06331900
C	-1.41394200	1.60690500	-1.14799300
C	-2.24144800	1.04622800	-0.00046100
C	-1.41431000	1.60693900	1.14731500
C	-0.73236700	0.83243300	2.06287700
C	0.61043100	1.40369500	2.19578800
C	1.77358100	0.53135900	2.10763300
C	2.59477600	1.10801000	1.12730900
C	3.04467000	0.34556200	0.00041700
C	2.59513700	1.10797400	-1.12663900
C	1.77427100	0.53129300	-2.10722500
C	0.61115400	1.40362800	-2.19579900
C	0.74740300	2.58365100	-1.42935800
C	-0.47245100	2.65726200	-0.69262800
C	-0.47268000	2.65729400	0.69223000
C	0.74692900	2.58370000	1.42936100
C	1.98184100	2.40903100	0.68143200
C	1.98207500	2.40901700	-0.68101700
C	0.07069700	-2.58010600	-1.42359000
C	1.25402600	-2.70659400	-0.71205100
C	1.25379700	-2.70656500	0.71243300
C	0.07023400	-2.58006100	1.42360100
C	-1.17257100	-2.43402400	0.70942400
C	-1.17234000	-2.43406800	-0.70983900
N	-4.92354300	-0.36572400	-0.00008000
H	-3.71175700	-0.63625900	-0.00047200
H	-5.27419500	-0.83302000	-0.83565500
H	-5.27353300	-0.83341400	0.83555600
B	-5.01520500	1.12725600	0.00033500
H	-3.31595700	1.45358500	-0.00064600
H	-5.15517900	1.65898300	-1.05191500
H	-5.15389600	1.65844500	1.05302700

 $C_{36}^{5-5}ts$

0 1

C	1.27067700	-0.06671900	-2.43775000
C	2.49157400	0.31438500	-1.78902500

C	2.45706200	1.39014800	-0.85406200
C	2.97469100	0.94153000	0.41024000
C	2.16934100	1.08493000	1.59123500
C	2.01979500	-0.18616000	2.22278500
C	0.69295700	-0.67839100	2.46058500
C	0.54355200	-1.94203100	1.81492200
C	-0.51711200	-2.13744400	0.87263000
C	0.04407400	-2.56301100	-0.37324100
C	-0.22712300	-1.82829200	-1.57278500
C	1.01384400	-1.44309100	-2.16839300
C	0.16442800	0.85154400	-2.46751300
C	-1.16434100	0.34019500	-2.16291600
C	-1.32411700	-0.91005200	-1.60842000
C	-2.30279100	-0.82971800	-0.43603600
C	-1.61985200	-1.22537200	0.87358300
C	-1.62265200	-0.15041000	1.73759600
C	-0.41499300	0.23680900	2.45392700
C	-0.19466900	1.58961600	2.15095100
C	1.05309600	1.98894000	1.57338800
C	0.74318500	2.67835600	0.36242600
C	1.34026700	2.29370200	-0.87526000
C	0.27036600	2.08244500	-1.80301300
C	-1.02960700	2.41017500	-1.13280500
C	-1.88583600	1.33142900	-1.33552800
C	-2.59738000	0.67250600	-0.28348100
C	-2.14990900	1.03245800	1.02578400
C	-1.31252300	2.11021300	1.30066700
C	-0.71284300	2.75037600	0.19893800
C	2.98606900	-0.86537500	-1.05805300
C	3.29008100	-0.47503600	0.27183900
C	2.70139100	-1.16661300	1.36255500
C	1.81373700	-2.23355100	1.12310500
C	1.50501700	-2.60543300	-0.20468100
C	2.10059200	-1.93247100	-1.29446100
N	-5.10291000	-0.35654000	0.29463300
H	-5.97263300	0.00301200	-0.10334000
H	-4.31152300	0.34623700	0.03392900
H	-5.17123400	-0.34158200	1.31453900
B	-4.70011200	-1.73357600	-0.28493000
H	-4.49113800	-2.59247500	0.50386000
H	-5.03855000	-1.90587500	-1.40975900
H	-3.21429500	-1.50917500	-0.67542000

$C_{36}^{6-5}ts$

0 1			
C	1.68905400	1.38845000	1.80737700
C	1.81062400	0.06118500	2.32104100
C	0.66122300	-0.78374300	2.40292500
C	0.94249600	-1.97880500	1.68634100
C	0.07560000	-2.40670800	0.63476200
C	0.85895300	-2.56561400	-0.54071900
C	0.50584800	-1.86108600	-1.72530500
C	1.63951600	-1.09444300	-2.13208600

C	1.52571000	0.31082800	-2.32370700
C	2.50927200	0.94512900	-1.50497000
C	2.11708100	1.93099600	-0.54779900
C	2.61468900	1.54293500	0.73187500
C	0.38080900	1.98178500	1.70698800
C	0.01585900	2.66663300	0.52351800
C	0.80426400	2.51546000	-0.64931400
C	-0.07025500	2.06514400	-1.68503700
C	0.21769100	0.89652300	-2.43162700
C	-0.93399500	0.06156400	-2.29492100
C	-0.80836100	-1.27860700	-1.82628700
C	-1.71327600	-1.41746900	-0.74360800
C	-1.24020500	-1.82595100	0.52553300
C	-1.62205300	-0.80549200	1.44679400
C	-0.64858600	-0.19838300	2.29565400
C	-0.75955000	1.19704700	2.08166700
C	-1.87496700	1.45334000	1.14287300
C	-1.42414200	2.37079200	0.19846900
C	-1.45811400	1.97178200	-1.15582900
C	-2.01121200	0.76428700	-1.57442700
C	-2.55112900	-0.15532900	-0.60047600
C	-2.48341100	0.21296200	0.80091100
C	2.85364100	-0.64372500	1.54200200
C	2.32287000	-1.88676500	1.15138000
C	2.27569800	-2.24491400	-0.20873500
C	2.74948000	-1.34928400	-1.17997400
C	3.28203300	-0.10066100	-0.80096900
C	3.32208200	0.25414100	0.56103800
H	-5.77240800	-0.94472700	1.43302900
H	-5.88412900	0.50032100	0.64047300
N	-5.32368900	-0.34603400	0.74062900
B	-5.08453300	-1.09049800	-0.65000000
H	-5.88279300	-0.74069300	-1.47137200
H	-4.89548700	-2.25834000	-0.45905200
H	-4.38553600	-0.06155200	1.12374300
H	-3.94259500	-0.58430300	-1.01337300

C_{36}^{5-5}

01

C	0.75717900	0.06971900	2.50587800
C	1.67395600	-0.93510000	2.04161000
C	1.16335100	-1.99993600	1.23562600
C	1.89285300	-2.04786500	-0.01533400
C	1.16443500	-1.97995200	-1.26556000
C	1.67639500	-0.90308000	-2.05518200
C	0.75962700	0.10920400	-2.50379400
C	1.20003100	1.37056800	-2.01279600
C	0.31684300	2.18475900	-1.22020800
C	0.96494200	2.49117100	0.01987100
C	0.31578600	2.16498500	1.25504200
C	1.19796500	1.33867000	2.03453200
C	-0.65067500	-0.20265300	2.51333900
C	-1.55774900	0.81620100	1.96945400

C	-1.08260900	1.89803000	1.25018100
C	-1.95599700	2.18900100	0.01675900
C	-1.08140200	1.91770700	-1.22059600
C	-1.55613600	0.84746700	-1.95725500
C	-0.64848600	-0.16303900	-2.51646500
C	-1.11587400	-1.38164400	-2.03035400
C	-0.23636800	-2.22934400	-1.26614500
C	-0.89573300	-2.47915300	-0.01991600
C	-0.23746300	-2.24925900	1.23110300
C	-1.11746900	-1.41366900	2.00738600
C	-2.38073700	-1.18023900	1.24024900
C	-2.60531800	0.18161300	1.21955900
C	-3.01056700	1.00848300	0.00689700
C	-2.60445100	0.20114200	-1.21859600
C	-2.37967800	-1.16035700	-1.26047900
C	-2.18558900	-1.81549300	-0.01527200
C	2.69612400	-0.26027100	1.24014600
C	2.81633300	-0.95087800	-0.00645700
C	2.69739200	-0.24109100	-1.24239800
C	2.41871500	1.13529200	-1.22803200
C	2.24754800	1.79833100	0.01465900
C	2.41762100	1.11574800	1.24696000
H	-2.39422800	3.19216100	0.02424400
H	-4.05456400	1.33740900	0.00928800

C_{36}^{6-6}

0 1

C	0.41633000	-2.62152000	-0.00107500
C	1.14659900	-2.18912700	-1.16760300
C	0.54278000	-1.39254200	-2.14946000
C	1.39937800	-0.20899100	-2.36122700
C	0.86835700	1.06399900	-2.13845600
C	1.68998800	1.79143100	-1.17063600
C	1.13690100	2.61768300	0.00184600
C	1.68823600	1.78933200	1.17356300
C	0.86504100	1.06149300	2.14085300
C	1.39564600	-0.21149700	2.36201600
C	0.53974600	-1.39550600	2.14856200
C	1.14488500	-2.19080000	1.16704800
C	-0.99797400	-2.53114600	-0.00195800
C	-1.62762000	-1.89913300	1.12547500
C	-0.87958900	-1.24660900	2.11571200
C	-1.45114200	0.09779100	2.20033600
C	-0.55765400	1.25833300	2.05764300
C	-1.13047000	2.10007000	1.13006300
C	-0.42163800	2.84979100	0.00114400
C	-1.12888500	2.10055000	-1.12874700
C	-0.55465700	1.26012500	-2.05687300
C	-1.44773300	0.09989700	-2.20081200
C	-0.87646800	-1.24461800	-2.11837000
C	-1.62552300	-1.89795200	-1.12910500
C	-2.73173000	-0.98926900	-0.68360400
C	-2.73337500	-0.99076300	0.67998300

C	-2.62095400	0.25084600	1.44092700
C	-2.38035700	1.45062200	0.69089200
C	-2.38036700	1.45154400	-0.69241000
C	-2.61964600	0.25251800	-1.44370800
C	2.36258500	-1.47302500	-0.72528300
C	2.55004100	-0.32895300	-1.46294000
C	2.67226400	0.93267500	-0.72823000
C	2.67188000	0.93189600	0.73208300
C	2.54812500	-0.33057100	1.46499400
C	2.36209000	-1.47406500	0.72661300
H	-0.62476000	3.92522200	0.00119700
H	1.61422500	3.60774600	0.00326400

C_{36}^{6-5}

0 1

C	0.93270800	-2.09281500	-1.24545300
C	1.72716100	-1.08769900	-1.88350300
C	1.09094400	0.09888500	-2.37053700
C	1.72728700	1.24096300	-1.78650700
C	0.93275500	2.18943800	-1.06709100
C	1.45224800	2.30501700	0.25494900
C	0.59864300	2.07927500	1.38034300
C	1.18499000	1.06474100	2.18434100
C	0.43624200	-0.10422700	2.49996600
C	1.18513400	-1.24309100	2.08808100
C	0.59879300	-2.18747900	1.20280000
C	1.45232700	-2.31842200	0.06219300
C	-0.49090300	-2.09998500	-1.44077300
C	-1.34890700	-2.24758900	-0.29661800
C	-0.82775300	-2.16991700	1.01901300
C	-1.62099600	-1.20431200	1.69793700
C	-0.99600500	-0.09645200	2.31335900
C	-1.62097900	1.05881000	1.79222200
C	-0.82776400	2.07751000	1.19604000
C	-1.34887500	2.26473300	-0.10864100
C	-0.49101500	2.21311500	-1.26124000
C	-1.08092600	1.23800900	-2.08811500
C	-0.33592100	0.10560900	-2.53275500
C	-1.08089200	-1.05992400	-2.18390600
C	-2.36749400	-0.65892800	-1.52771500
C	-2.54666500	-1.40765600	-0.40819400
C	-2.90721100	-0.83226700	0.94362400
C	-2.90714400	0.75078900	1.00963400
C	-2.54646200	1.43657900	-0.28960600
C	-2.36738600	0.78370100	-1.46755000
C	2.76843200	-0.66570900	-0.93517000
C	2.76852600	0.74147900	-0.87642000
C	2.61371400	1.39679300	0.36994800
C	2.45080900	0.64372900	1.54091800
C	2.45074300	-0.76993500	1.48175100
C	2.61373800	-1.42277200	0.25215500
H	-3.81574600	-1.24299300	1.39231200
H	-3.81563700	1.12301500	1.49081900

Li@C₆₀

1 1

C	-0.43072900	3.07975400	1.69458300
C	-1.77037200	2.83707600	1.18920300
C	-2.53010400	1.80263300	1.71541000
C	-1.98805800	0.96694000	2.77240300
C	-0.71166600	1.20273700	3.26007900
C	0.08523900	2.28312100	2.70691000
C	0.40772300	3.46717800	0.57380100
C	-0.41315300	3.46180200	-0.62423400
C	-1.75935400	3.07289000	-0.24303500
C	-2.50828100	2.26345900	-1.08457500
C	-3.31661000	0.95765000	0.83493400
C	-2.44038300	-0.39405200	2.54483200
C	-1.59573000	-1.46093400	2.81299800
C	-0.25621500	-1.21435200	3.31643400
C	0.17453000	0.08618800	3.53695400
C	1.51925900	0.47537700	3.15278600
C	1.46420900	1.83428100	2.63947900
C	2.27101600	2.21259900	1.57283600
C	1.72995200	3.04737300	0.51424800
C	0.12011900	3.02953100	-1.83064400
C	1.49914600	2.57997100	-1.89134600
C	2.28859000	2.59425100	-0.74803600
C	3.18309500	1.47810900	-0.47171600
C	3.17222800	1.24141700	0.96720300
C	3.22558600	-0.06460600	1.46086000
C	2.37963200	-0.45442000	2.58121000
C	1.92862600	-1.81629200	2.35200300
C	0.63755400	-2.18418700	2.70840700
C	-3.26111000	-0.39929800	1.34735300
C	-0.43576800	-3.47326200	-0.57505000
C	-1.75122600	-3.03960400	-0.51327200
C	-2.29357500	-2.20411100	-1.57028700
C	-1.49521700	-1.83569800	-2.64291400
C	-0.11516100	-2.28309800	-2.70444900
C	1.73959700	-2.83572000	-1.19050600
C	1.72870600	-3.07170000	0.24394100
C	0.38388000	-3.46643600	0.62365200
C	-0.14947400	-3.02891000	1.82811300
C	-1.52932900	-2.58215200	1.89353200
C	-2.31059300	-2.58559000	0.74772800
C	-3.18710400	-1.23472900	-0.96301000
C	-3.23996600	0.06170300	-1.45312400
C	-2.40096300	0.44816700	-2.57310200
C	-1.54998600	-0.47904300	-3.15534200
C	-0.20423900	-0.08695800	-3.53359000
C	0.68316800	-1.20240500	-3.25557800
C	1.96768000	-0.97114600	-2.78109200
C	2.50817900	-1.80805500	-1.72407300
C	2.48665100	-2.27127000	1.09036000
C	3.29189200	-1.19138700	0.53690600
C	3.30212400	-0.96431300	-0.84134800

C	3.24685700	0.39922500	-1.35648000
C	2.41925700	0.39084700	-2.55516500
C	1.56533400	1.45668300	-2.81193300
C	0.22671600	1.21442300	-3.31921400
C	-0.66570000	2.18606600	-2.71293500
C	-1.94914300	1.80984000	-2.34587800
C	-3.19790100	-1.47062900	0.46886200
C	-3.30625200	1.18314000	-0.53376800
C	0.40123900	-3.08434900	-1.69601600
Li	1.45116200	0.06854900	0.02738100

$Li@C_{60}^{AB}$

1 1

C	0.78738200	2.45205200	-2.28923600
C	-0.64465800	2.69193100	-2.29145500
C	-1.25808700	3.22373800	-1.16659300
C	-0.46896900	3.54258100	0.01033900
C	0.89955300	3.31855600	0.01125400
C	1.54163200	2.75847700	-1.16484500
C	1.03757200	1.22238900	-3.01779700
C	-0.24077600	0.70106500	-3.46970900
C	-1.28029100	1.61012200	-3.02031000
C	-2.50060200	1.10826000	-2.59190300
C	-2.53689500	2.70156300	-0.72037300
C	-1.26079100	3.21683000	1.18353700
C	-0.64995800	2.67833600	2.30667500
C	0.78208700	2.43853000	2.30630500
C	1.53897000	2.75155000	1.18545400
C	2.57838900	1.84324400	0.73609900
C	2.58002900	1.84756400	-0.71841000
C	2.82541500	0.67390500	-1.41907000
C	2.03578300	0.35350500	-2.59501100
C	-0.46989000	-0.66728900	-3.47662300
C	0.56983100	-1.57618000	-3.02613900
C	1.79591300	-1.07962100	-2.60121600
C	2.44226500	-1.65053900	-1.42645500
C	3.07991500	-0.56392900	-0.69483300
C	3.07838500	-0.56808900	0.69939200
C	2.82218600	0.66545200	1.43038300
C	2.02981100	0.33815800	2.60257300
C	1.03061200	1.20455000	3.02811200
C	-2.53854300	2.69727700	0.73128500
C	-1.75526500	-1.20996700	3.02072100
C	-2.74497300	-0.33927000	2.58899500
C	-3.53392700	-0.65905000	1.41294800
C	-3.29748700	-1.83521100	0.71699400
C	-2.25788400	-2.74429300	1.16452600
C	-0.07358300	-2.67798600	2.28922900
C	0.56289400	-1.59405900	3.01886900
C	-0.47788200	-0.68780900	3.47229600
C	-0.24876900	0.68056500	3.47406500
C	-1.28725500	1.59222700	3.02760300
C	-2.50656400	1.09290400	2.59333900

C	-3.78338800	0.57621600	0.69119300
C	-3.78178400	0.58034000	-0.69572400
C	-3.53061600	-0.65061800	-1.42419400
C	-3.29576800	-1.83085500	-0.73464400
C	-2.25519000	-2.73735100	-1.18507600
C	-1.61451700	-3.30275700	-0.01121600
C	-0.24616800	-3.54051200	-0.01033700
C	0.54193700	-3.22172300	1.16802700
C	1.78994900	-1.09501900	2.59978900
C	2.43906500	-1.65901000	1.42314100
C	1.82845600	-2.70234400	0.72346000
C	1.83007900	-2.69800700	-0.73439500
C	0.54461300	-3.21479500	-1.18497100
C	-0.06830800	-2.66443600	-2.30443100
C	-1.50012000	-2.42568100	-2.30729600
C	-1.74831200	-1.19213000	-3.03107600
C	-2.73899000	-0.32395600	-2.59651600
C	-3.14761800	1.65861800	1.42047700
C	-3.14440300	1.66705900	-1.41716000
C	-1.50541400	-2.43922000	2.29025300
N	7.69417100	0.12615500	-0.00065400
H	8.20688800	-0.75575700	-0.00461300
H	7.98521600	0.65543000	-0.82266500
H	7.98797000	0.64967900	0.82405900
B	6.07459000	-0.13657400	0.00093400
H	5.84691400	-0.77118800	1.00839200
H	5.56308900	0.96474500	0.00486700
H	5.84429400	-0.76510700	-1.00984700
Li	0.91300700	-0.73105400	-0.00073700

$Li@C_{60}^{6-6}ts1$

1 1

C	-0.20969300	3.54333200	0.07168300
C	0.96102200	3.18255600	0.85570600
C	2.06095800	2.59544300	0.24102000
C	2.04542000	2.34373200	-1.18952000
C	0.92583200	2.68888500	-1.93709100
C	-0.22647700	3.29920900	-1.29184900
C	-1.38629600	3.26655900	0.87490200
C	-0.94249000	2.73952400	2.15285900
C	0.50767700	2.68875300	2.13727700
C	1.17467200	1.63356100	2.75012100
C	2.77378600	1.51423400	0.88650800
C	2.74644400	1.10583800	-1.44271900
C	2.26607500	0.23563300	-2.40211400
C	1.09747400	0.58488900	-3.18411100
C	0.44256200	1.78901800	-2.95903500
C	-1.00808700	1.83684200	-2.95306400
C	-1.42213300	2.76981000	-1.92093500
C	-2.54706000	2.50073500	-1.15388400
C	-2.52828100	2.75368000	0.27552000
C	-1.66041000	1.72650700	2.77351300
C	-2.85887000	1.19763800	2.15209700

C	-3.27992400	1.69760900	0.92787100
C	-3.76694700	0.79409300	-0.09917200
C	-3.31075800	1.28883400	-1.38536800
C	-2.91465300	0.39738800	-2.37229000
C	-1.73618600	0.67618600	-3.16961200
C	-1.05024300	-0.58249700	-3.41014800
C	0.33550000	-0.62606500	-3.41945000
C	3.36341900	0.61345900	-0.16157900
C	0.74149000	-3.25649800	-0.88739900
C	1.88693700	-2.74227000	-0.28337300
C	1.90974400	-2.49384600	1.14202300
C	0.77942500	-2.76098600	1.91257700
C	-0.41675300	-3.29783200	1.28448500
C	-1.60443900	-3.18884300	-0.86805200
C	-1.14571100	-2.69358800	-2.15378400
C	0.30535400	-2.74556300	-2.16547000
C	1.03471600	-1.73023500	-2.78075500
C	2.23536700	-1.21120500	-2.17032300
C	2.64239800	-1.68748700	-0.93046800
C	2.69573900	-1.28749300	1.37659900
C	2.31003100	-0.40873800	2.39486400
C	1.11447400	-0.68031700	3.16971900
C	0.37109100	-1.83973200	2.95163500
C	-1.07997400	-1.78883800	2.95842800
C	-1.56690500	-2.69433100	1.93278200
C	-2.68118700	-2.35231000	1.18050100
C	-2.70116700	-2.60561700	-0.25018700
C	-1.80924200	-1.63950200	-2.76447600
C	-2.95739100	-1.03180400	-2.11908300
C	-3.39624400	-1.50489500	-0.89073800
C	-3.80619600	-0.57103600	0.14241500
C	-3.36527300	-1.09543100	1.42268800
C	-2.90171700	-0.23206200	2.40489600
C	-1.73438100	-0.58682600	3.18971600
C	-0.96316700	0.62339200	3.41302500
C	0.42447600	0.57997300	3.40530900
C	3.19661900	-0.80866500	0.09556300
C	2.33213700	1.03159100	2.10956900
C	-0.43460300	-3.53787100	-0.08188200
N	6.19876500	-0.67276400	-0.08678800
H	6.88777400	-1.02971600	0.57887300
H	6.50955200	-0.93026600	-1.02561700
H	5.30658700	-1.17144900	0.09872500
B	5.98472100	0.89250900	0.08192700
H	4.69224900	0.99128600	-0.26326500
H	5.98777900	1.20350300	1.23454300
H	6.55409000	1.52376500	-0.75324700
Li	1.04637000	-0.14647600	0.53340500

$Li@C_{60}^{6-}ts_2$

11

C	-1.99838400	-2.81866200	-1.30219900
C	-0.70046600	-2.91680200	-1.95425600

C	0.43666100	-3.22267300	-1.20909200
C	0.31963400	-3.45131800	0.22184300
C	-0.92623900	-3.36751500	0.84029400
C	-2.10956500	-3.04021600	0.05972800
C	-2.72510400	-1.72746700	-1.92326500
C	-1.87660100	-1.15754700	-2.95464200
C	-0.63139400	-1.89937500	-2.97070600
C	0.57138000	-1.23245600	-3.18384800
C	1.69705300	-2.57156000	-1.46296400
C	1.50893600	-2.94621400	0.86328600
C	1.38717100	-2.30462300	2.08034000
C	0.09530000	-2.18775000	2.72404500
C	-1.04140800	-2.72115600	2.12240700
C	-2.28970000	-1.98319900	2.14804500
C	-2.95112400	-2.18098500	0.87118300
C	-3.64109700	-1.13121100	0.28053800
C	-3.52531500	-0.89934900	-1.14839200
C	-1.86552500	0.21616100	-3.15856700
C	-2.70628000	1.07896200	-2.35557200
C	-3.51765100	0.53417700	-1.37013600
C	-3.63360200	1.18960600	-0.08045400
C	-3.70539000	0.15901100	0.93971800
C	-3.07426900	0.34652600	2.16212000
C	-2.34764600	-0.74534200	2.77472600
C	-1.16192700	-0.19289900	3.40936400
C	0.03111700	-0.89979500	3.38604700
C	2.58316200	-2.59732100	-0.19471000
C	2.11190200	1.74638200	1.92749200
C	2.91056800	0.91275800	1.14315700
C	3.03720100	1.14646300	-0.28364200
C	2.33960000	2.20811200	-0.88813800
C	1.50003700	3.06828200	-0.06725100
C	0.09841700	2.94634200	1.95187100
C	0.03102900	1.91270000	2.97103500
C	1.28547500	1.18313400	2.96010600
C	1.29099200	-0.20489500	3.15370100
C	2.14582300	-1.06340900	2.37855700
C	2.92632700	-0.52161500	1.35650700
C	3.07164600	-0.15247500	-0.92041900
C	2.49521400	-0.32367400	-2.17402000
C	1.76764300	0.75295400	-2.76697400
C	1.70198200	2.01365400	-2.15226500
C	0.44421500	2.74461900	-2.13508400
C	0.32338900	3.40430500	-0.84719600
C	-0.91406800	3.49268100	-0.22463600
C	-1.02917900	3.25864200	1.20473400
C	-1.16507200	1.24580500	3.19858300
C	-2.34124900	1.57555600	2.42054500
C	-2.27796300	2.56190700	1.44598400
C	-2.93548100	2.36248100	0.16705700
C	-2.09106900	2.93804200	-0.86438200
C	-1.97412300	2.30839900	-2.09588700
C	-0.68148500	2.20941400	-2.74134200
C	-0.60965100	0.90789300	-3.39220300
C	0.57980800	0.19948500	-3.40730300

C	3.20736100	-1.20333500	0.08568000
C	1.74216400	-1.57600900	-2.41218700
C	1.38837900	2.84393500	1.29756800
N	5.84655500	-0.34032900	0.17786300
H	6.19163900	-0.42378300	1.13647100
H	6.44006600	-0.90096600	-0.43887800
H	4.82023500	-0.88861900	0.15669100
B	5.69055700	1.08930600	-0.30213700
H	5.68695000	1.93557900	0.52262800
H	5.73123000	1.25725200	-1.47174300
Li	0.97502200	-0.67249200	0.39731600
H	3.33676900	-3.39146500	-0.25865000

Li@C₆₀⁻⁶1

1 1

C	-2.43872700	2.50847500	1.28214900
C	-1.17302600	2.84858100	1.91693300
C	-0.11517900	3.32633100	1.14922100
C	-0.28442700	3.49224100	-0.28509300
C	-1.50558300	3.19223900	-0.88638700
C	-2.60342700	2.68039000	-0.08099400
C	-2.95421000	1.31844200	1.93412700
C	-2.00561500	0.93078200	2.96282300
C	-0.91468000	1.88022200	2.95164800
C	0.38986900	1.43703600	3.15803900
C	1.23755200	2.90313900	1.40000200
C	0.95858300	3.17380000	-0.93118300
C	0.94870400	2.51634100	-2.14672600
C	-0.31331400	2.17002600	-2.76514000
C	-1.52000500	2.51062700	-2.15378500
C	-2.61937000	1.56505800	-2.14570700
C	-3.28980500	1.66877200	-0.86468600
C	-3.77805800	0.52580900	-0.24464200
C	-3.60525700	0.34779900	1.18650400
C	-1.74659600	-0.41759200	3.18552200
C	-2.43530900	-1.43186700	2.41120100
C	-3.34539800	-1.05863300	1.43289000
C	-3.36348900	-1.75182500	0.15724200
C	-3.62387400	-0.76801100	-0.87990400
C	-2.98686400	-0.86682000	-2.10919400
C	-2.46930900	0.32147100	-2.75010700
C	-1.21306500	-0.02939400	-3.39281400
C	-0.16125300	0.87880100	-3.41201400
C	2.07425100	3.01787900	0.11579700
C	2.37352800	-1.33380600	-1.92024400
C	3.03466300	-0.37317800	-1.17360000
C	3.41104200	-0.57088800	0.26200300
C	2.67818100	-1.69275300	0.88931800
C	2.00962200	-2.71303700	0.10190400
C	0.59531500	-2.87373700	-1.89533000
C	0.33664700	-1.88181600	-2.92622200
C	1.44139800	-0.94401600	-2.95178600

C	1.21426900	0.42463900	-3.20120700
C	1.91639200	1.43236200	-2.45398400
C	2.76704100	1.02674300	-1.40862800
C	3.03670900	0.76113800	0.86134500
C	2.44540700	0.85848600	2.14873500
C	1.92435900	-0.29836600	2.74110000
C	2.06159800	-1.58666300	2.12841000
C	0.94127200	-2.53582000	2.16593700
C	0.91968400	-3.24201900	0.90200000
C	-0.29052800	-3.55442400	0.30053000
C	-0.45910400	-3.36531400	-1.12946200
C	-0.96411400	-1.44338100	-3.15654000
C	-2.05366100	-1.95707100	-2.35790900
C	-1.80884500	-2.89910700	-1.36587700
C	-2.47924000	-2.79244600	-0.08048800
C	-1.53710700	-3.19610000	0.94714700
C	-1.50994600	-2.52457100	2.16238200
C	-0.24292500	-2.18943000	2.77691600
C	-0.38896800	-0.86836600	3.40412200
C	0.65389600	0.03758700	3.39467400
C	2.80436400	1.71036600	-0.12949500
C	1.47758500	1.95821300	2.36719800
C	1.85175400	-2.54474000	-1.26253300
N	5.89127100	0.30658800	-0.23577200
H	5.78720500	0.31298900	-1.25308600
H	6.88743700	0.19707400	-0.03327200
Li	0.60812000	0.41619000	-1.07267100
H	2.73921000	3.89266200	0.13370700
H	5.60647500	1.22675600	0.11146900
B	5.07920200	-0.90820000	0.47304400
H	5.35922100	-1.91501400	-0.11509600
H	5.34073700	-0.87977300	1.64265500

$Li@C_{60}^{6-6}$

1 1

C	0.02719800	3.48507600	-0.68375900
C	-1.17007600	3.02633600	-1.36965800
C	-2.26373500	2.57394500	-0.63292200
C	-2.21827400	2.57594100	0.81793500
C	-1.07488400	3.02514800	1.47204800
C	0.07271100	3.47709300	0.70181700
C	1.17384000	3.03657300	-1.44978400
C	0.68101800	2.30502500	-2.60545700
C	-0.77065000	2.30716000	-2.55262300
C	-1.49634300	1.18038100	-2.95490800
C	-3.02556200	1.43129800	-1.05607100
C	-2.95120200	1.43370100	1.29016000
C	-2.47751900	0.74171500	2.37389200
C	-1.27972300	1.17574000	3.05150800
C	-0.59307300	2.30806900	2.62321900
C	0.85666800	2.30325000	2.57721400
C	1.26967400	3.02991800	1.38949000
C	2.36721000	2.59839900	0.65708800

C	2.31654900	2.59811700	-0.79437500
C	1.35720300	1.17672600	-3.05478300
C	2.55591200	0.72658300	-2.37586400
C	3.02233000	1.42033500	-1.26700900
C	3.50979800	0.69397100	-0.10867500
C	3.10449000	1.42264200	1.07922600
C	2.70811600	0.72738900	2.21304500
C	1.56074200	1.17589900	2.97583600
C	0.84532400	0.00027700	3.44075800
C	-0.54073000	0.00029000	3.47187300
C	-3.73168200	0.79187500	0.14064200
C	-1.07492400	-3.02488800	1.47254800
C	-2.21830700	-2.57577100	0.81835700
C	-2.26376800	-2.57400500	-0.63250000
C	-1.17012000	-3.02653900	-1.36916500
C	0.02714800	-3.48518200	-0.68318800
C	1.26963100	-3.02970600	1.38998700
C	0.85663600	-2.30283800	2.57759400
C	-0.59310700	-2.30762800	2.62360300
C	-1.27974200	-1.17521700	3.05170200
C	-2.47753000	-0.74128600	2.37401600
C	-2.95121300	-1.43344200	1.29039100
C	-3.02558100	-1.43141600	-1.05583700
C	-2.64518400	-0.74444100	-2.18699400
C	-1.49637500	-1.18085000	-2.95474500
C	-0.77068900	-2.30756600	-2.55225500
C	0.68098500	-2.30546000	-2.60508200
C	1.17379600	-3.03682100	-1.44928600
C	2.31651300	-2.59827200	-0.79394900
C	2.36717200	-2.59831900	0.65751300
C	1.56072600	-1.17543000	2.97602800
C	2.70810500	-0.72706100	2.21316300
C	3.10447100	-1.42250600	1.07946000
C	3.50979000	-0.69403400	-0.10856100
C	3.02231000	-1.42057800	-1.26677700
C	2.55590200	-0.72700100	-2.37574600
C	1.35718200	-1.17723900	-3.05458700
C	0.60814400	-0.00028300	-3.47096600
C	-0.78574500	-0.00027300	-3.43382800
C	-3.73168000	-0.79178900	0.14077000
C	-2.64516900	0.74412500	-2.18710800
C	0.07266300	-3.47697700	0.70238700
Li	-0.61024200	-0.00038600	-1.22418000
H	-4.77676000	-1.12042100	0.16595100
H	-4.77675800	1.12051100	0.16574700

$Li@C_{60}^{6-5}ts$

11

C	0.84508900	1.84114800	2.76113400
C	-0.30004800	2.62743100	2.34603600
C	-1.58099000	2.12494100	2.51427900
C	-1.77559900	0.81580600	3.11469800
C	-0.68070100	0.07002100	3.52855400

C	0.65963800	0.59470300	3.34872300
C	1.91234300	2.04983300	1.80968100
C	1.42058100	3.00079200	0.79079800
C	0.05529000	3.33084200	1.12224900
C	-0.90405100	3.50219200	0.12053600
C	-2.57560900	2.29463000	1.46744000
C	-2.88099000	0.17243100	2.43404200
C	-2.83821100	-1.19379300	2.18278700
C	-1.69248200	-1.97423900	2.60994400
C	-0.63776700	-1.35839300	3.26932600
C	0.72936500	-1.70824200	2.93491800
C	1.52402400	-0.49551900	2.97406500
C	2.54395500	-0.28618000	2.04246300
C	2.76238300	1.01848900	1.47335700
C	1.79657000	2.80811100	-0.53508600
C	2.69340900	1.72325800	-0.91606700
C	3.43216000	0.89869100	0.09922700
C	3.33116500	-0.63354000	-0.19164000
C	2.80694000	-1.28322700	1.03083200
C	2.04841400	-2.43746600	0.99359100
C	0.98255900	-2.65199200	1.95343400
C	-0.11822500	-3.30761900	1.26944800
C	-1.42556600	-2.97156500	1.58863300
C	-3.37109500	1.08023600	1.41409900
C	-2.53672700	-2.08423800	-1.81368100
C	-3.36990800	-1.03348300	-1.46033700
C	-3.17499300	0.27625100	-2.05434400
C	-2.15656800	0.47630000	-2.97444100
C	-1.27848600	-0.62269000	-3.34096100
C	-0.32554500	-2.65304600	-2.35524900
C	-0.67974200	-3.34189900	-1.12555700
C	-2.04835800	-2.99562200	-0.79189300
C	-2.40995400	-2.81047900	0.53382800
C	-3.28520500	-1.71124500	0.90430700
C	-3.75006000	-0.84144900	-0.07146200
C	-3.44203800	1.27830400	-1.03456700
C	-2.69030000	2.44230000	-0.98230200
C	-1.62048800	2.65154400	-1.94340000
C	-1.36029200	1.68832500	-2.91257500
C	0.01065700	1.33134700	-3.22815100
C	0.05902800	-0.09878000	-3.51528900
C	1.16249400	-0.83459500	-3.10383200
C	0.95823500	-2.14731000	-2.51639600
C	0.26206800	-3.49802100	-0.11759600
C	1.59410600	-2.95043800	-0.29106900
C	1.93388300	-2.29899000	-1.46264200
C	2.73038000	-1.07709700	-1.40995500
C	2.29448200	-0.20430500	-2.44006600
C	2.22701900	1.18661800	-2.12499800
C	1.06351900	1.96808400	-2.58345800
C	0.79946600	2.97951300	-1.58530500
C	-0.52296900	3.31023100	-1.25832200
C	-3.79821200	0.58402800	0.19006700
C	-2.24330200	2.96124300	0.29867100
C	-1.47340600	-1.87990200	-2.78057000

N	6.00852200	-0.72691600	-0.13759300
H	4.77855700	-0.86333800	-0.24545800
H	6.37898100	-1.00919200	-1.04650400
H	6.26590300	-1.42046700	0.56662300
B	6.26578700	0.69447300	0.24311300
H	6.51983100	1.45107100	-0.63370300
H	4.52385400	1.21389000	0.17104200
H	6.31718400	0.93981800	1.40239000
Li	0.55970200	1.03019900	-0.55551700

$Li@C_{60}^{6-5}ts_2$

1 1

C	-1.06593700	0.09464500	-3.43831000
C	-0.08397000	1.15078500	-3.33171600
C	1.25278500	0.85370200	-3.07058600
C	1.64134700	-0.54199000	-2.91996600
C	0.69416500	-1.55851300	-3.03175300
C	-0.68833300	-1.24115100	-3.30693800
C	-2.30672700	0.56267200	-2.83920000
C	-2.09759400	1.91386800	-2.34986100
C	-0.72309300	2.28196500	-2.63618700
C	-0.00788400	3.05541200	-1.73423500
C	2.05453400	1.66424100	-2.15524900
C	2.63587000	-0.59223900	-1.87636800
C	2.65477500	-1.65335100	-0.98708300
C	1.69009000	-2.72752800	-1.10338900
C	0.72255700	-2.67384400	-2.10030000
C	-0.64674600	-3.04817600	-1.80125000
C	-1.52086200	-2.15375900	-2.54277000
C	-2.69705400	-1.70366400	-1.96398800
C	-3.10022800	-0.31660900	-2.11744500
C	-2.69438500	2.32803600	-1.16218500
C	-3.52607700	1.40558700	-0.40880200
C	-3.71939500	0.11428900	-0.87466600
C	-3.69051400	-1.00729000	0.04836300
C	-3.05883900	-2.12601200	-0.62145000
C	-2.22579000	-2.98115700	0.08669400
C	-0.98757700	-3.44398500	-0.51677500
C	0.02211300	-3.50103500	0.52577900
C	1.33448000	-3.14942400	0.23953100
C	2.83933500	0.77442000	-1.38915900
C	1.70971700	-0.58259000	2.84773600
C	2.48921200	0.31263500	2.11461500
C	2.12775000	1.69606200	1.98608000
C	0.94032900	2.11860400	2.53958400
C	0.10803300	1.20298300	3.28012200
C	-0.49277100	-1.18497400	3.34437500
C	0.13589900	-2.31036300	2.67220500
C	1.50327300	-1.94137900	2.37086500
C	2.09057900	-2.34893500	1.18476600
C	2.92493300	-1.42625700	0.42926500
C	3.07280000	-0.11958300	0.86764400
C	2.74566700	2.30721700	0.71363800

C	1.64948900	2.98894800	-0.08785600
C	0.39293200	3.41839000	0.52256000
C	0.04369000	3.03664400	1.80365800
C	-1.31556900	2.65450900	2.09935100
C	-1.28038900	1.52791600	3.01666500
C	-2.22127600	0.51414100	2.91462500
C	-1.81710100	-0.87326800	3.07612400
C	-0.59121600	-3.07347700	1.76857900
C	-1.97811900	-2.74896300	1.49481900
C	-2.57903100	-1.67232600	2.13761500
C	-3.45261900	-0.78346900	1.39738900
C	-3.24194700	0.57042900	1.88398700
C	-3.27775100	1.64072500	1.00452800
C	-2.30335000	2.71186000	1.11600100
C	-1.94595400	3.13199600	-0.21772600
C	-0.62690000	3.48692900	-0.50484700
C	3.25688500	1.02175600	-0.03554600
C	1.41269000	2.74370700	-1.42992500
C	0.49083600	-0.12482800	3.45459300
N	5.89317600	0.33701700	-0.24136600
H	6.15041900	0.41654000	-1.22669100
H	6.45316600	0.98981300	0.31054400
H	4.73395300	0.80567700	-0.17834600
B	5.85866400	-1.05645500	0.29844500
H	5.75012200	-1.93944100	-0.48169400
H	5.99181700	-1.18363600	1.46707500
Li	0.25985900	0.92972800	-0.98936900
H	3.56477400	2.99540900	0.95720600

$Li@C_{60}^{6-5}$

11

C	-1.32658200	2.47679900	-2.21156200
C	-0.22255900	3.18560600	-1.60211200
C	1.08605800	2.80481500	-1.88503300
C	1.34063800	1.69635900	-2.76737500
C	0.29182100	1.02107600	-3.34522000
C	-1.07050800	1.41347300	-3.07137800
C	-2.39383100	2.36867900	-1.23345000
C	-1.93939600	3.00965800	-0.00938300
C	-0.59624400	3.51312700	-0.24342600
C	0.35793000	3.44062600	0.76552400
C	2.07401100	2.72885300	-0.82993500
C	2.50638500	0.96285200	-2.23283900
C	2.53231100	-0.48472900	-2.34386200
C	1.39776500	-1.16939300	-2.99726800
C	0.32167100	-0.45029100	-3.46136000
C	-1.02404500	-0.93623100	-3.26022300
C	-1.88049000	0.20945300	-3.00734900
C	-2.90479700	0.11411000	-2.07836100
C	-3.16046200	1.21583900	-1.16740500
C	-2.27989200	2.47183800	1.22092300
C	-3.08914900	1.26607200	1.29155900
C	-3.51773300	0.65161400	0.12331800

C	-3.48885800	-0.79273000	0.00725100
C	-3.11226800	-1.12854500	-1.35593800
C	-2.30295600	-2.22602900	-1.60463000
C	-1.23539700	-2.13254000	-2.58293800
C	-0.10183100	-2.88693400	-2.09031100
C	1.18956000	-2.41287600	-2.30392200
C	2.95797700	1.58481800	-1.10081300
C	2.29701800	-2.33147600	1.20349300
C	3.09045400	-1.20009200	1.14266400
C	2.81406100	-0.09994700	2.02908700
C	1.79903000	-0.19965400	3.00385000
C	0.99162000	-1.39902000	3.08055300
C	0.11991100	-3.15265500	1.56666700
C	0.49630700	-3.49757200	0.20710300
C	1.84108000	-3.01446300	-0.02947900
C	2.17868300	-2.46651500	-1.24683000
C	3.02000800	-1.26386500	-1.32959400
C	3.77873600	-0.71530900	-0.13960500
C	3.04314200	1.13601200	1.32958000
C	2.20178800	2.19988400	1.56554100
C	1.13751400	2.10610400	2.53676600
C	0.94201000	0.93478300	3.26328100
C	-0.40430400	0.44503200	3.49724800
C	-0.37664800	-1.00306300	3.38143700
C	-1.43704900	-1.67094800	2.77776600
C	-1.18353200	-2.77163400	1.85859500
C	-0.45940300	-3.44419800	-0.80421200
C	-1.82053500	-3.03646000	-0.49704900
C	-2.17883800	-2.71563200	0.80286200
C	-3.03505300	-1.56907400	1.06398100
C	-2.57854100	-0.92999900	2.28154400
C	-2.60273200	0.45947900	2.39219900
C	-1.49193700	1.15744000	3.00548300
C	-1.28575900	2.39891600	2.27629600
C	0.00039400	2.86619000	2.04953200
C	3.74383900	0.88809100	-0.01126700
C	1.71753500	3.05099700	0.45808600
C	1.23256800	-2.44122200	2.17991000
H	4.77644900	1.25240000	0.01459500
H	4.82541300	-1.03673500	-0.15981300
Li	0.79839100	-0.54289100	1.01247500

Li@C₇₀

1 1			
C	-3.21656700	-0.86177800	2.23255400
C	-2.44530700	-2.08342500	2.13791500
C	-3.96146000	-0.41781800	1.14362100
C	-2.46512900	-2.83859000	0.97210400
C	-1.22298600	-3.42177900	0.48094800
C	-0.01363200	-3.32962900	1.22462800
C	1.18702300	-3.42126500	0.47940100
C	-3.19471600	1.87868900	1.54315700
C	-2.41631200	1.40692000	2.67056600
C	-3.95372000	0.99149100	0.79269700

C	-2.43069400	0.07087900	3.01161900
C	-1.19597700	-0.58301100	3.40642700
C	0.01130800	0.14078800	3.55240700
C	1.20738000	-0.60340500	3.40112800
C	-0.00783100	-2.54809300	2.46993700
C	-1.20562800	-1.90710700	2.87367500
C	1.19898000	-1.92642400	2.87067900
C	-3.19298000	2.07378700	-1.27399800
C	-2.40650400	2.99600600	-0.48496400
C	-3.95330100	1.09186600	-0.65475500
C	-2.40740300	2.90105400	0.89068400
C	-1.16731300	3.06918800	1.62754700
C	0.03554700	3.42471600	0.97378800
C	1.23370300	3.04652700	1.62587800
C	0.02203900	1.56646000	3.19676600
C	-1.17454500	2.15475600	2.72167300
C	1.22754800	2.13283300	2.71890000
C	-3.21307000	-0.54516600	-2.33525400
C	-2.42638200	0.48597400	-2.97658800
C	-3.95967400	-0.25576300	-1.19709500
C	-2.41353200	1.76263700	-2.45512100
C	-1.17199300	2.51120100	-2.40044000
C	0.02534800	1.99312200	-2.94948700
C	1.23053400	2.48881500	-2.39831700
C	0.03634900	3.52673900	-0.49246200
C	-1.16612700	3.26543300	-1.19003100
C	1.23537700	3.24222500	-1.18875900
C	-3.24226800	-2.38168400	-0.16730200
C	-2.46076400	-2.67308600	-1.35593800
C	-3.96872400	-1.18788300	-0.08581500
C	-2.44059300	-1.76716200	-2.40708900
C	-1.20166400	-1.49257900	-3.11202300
C	-0.00497000	-2.18382300	-2.79935000
C	1.20186700	-1.51261600	-3.10881900
C	0.01518800	0.63003700	-3.49780600
C	-1.19145700	-0.10708000	-3.45597400
C	1.21077200	-0.12838900	-3.45114800
C	-0.01176200	-3.12831800	-1.67190800
C	-1.22098600	-3.31970700	-0.94871400
C	1.18779000	-3.32264100	-0.94551300
C	3.22563100	-0.59964000	-2.33470100
C	2.43659000	-1.80830900	-2.40641800
C	2.43246200	-2.69659800	-1.35056100
C	3.97207400	-0.32186200	-1.19685800
C	3.24421700	2.02126100	-1.27506100
C	2.46195100	1.72169500	-2.45377300
C	2.45553800	0.44416200	-2.97276100
C	3.98314400	1.02358700	-0.65488500
C	3.24318400	1.82595500	1.54413100
C	2.47138000	2.85879900	0.88995100
C	2.47202800	2.95401300	-0.48481400
C	3.98192300	0.92294200	0.79238800
C	3.22422200	-0.91604000	2.23211900
C	2.45237900	0.02988000	3.00601000
C	2.45923300	1.36629900	2.66863900

C	3.97124700	-0.48403100	1.14345100
C	3.21154600	-2.41709100	-0.16634100
C	2.43058800	-2.85527200	0.96745800
C	2.43513000	-2.12263200	2.13666900
C	3.96556500	-1.25247200	-0.08570700
Li	-1.34163100	-1.19713200	-0.02592500

Li@C₇₀^{AB}

1 1

C	-3.71310200	-0.09430400	-0.16209400
C	-3.23078100	-0.77497800	-1.35021900
C	-3.65624700	1.29962900	-0.08297200
C	-2.71106700	-0.03559400	-2.40229800
C	-1.52659100	-0.49653400	-3.10699600
C	-0.91444500	-1.73549400	-2.79388000
C	0.46205000	-1.84837800	-3.10500500
C	-2.84516200	1.16047900	2.23388100
C	-2.88196300	-0.28394200	2.14047500
C	-3.22027300	1.94075900	1.14444600
C	-3.31553300	-0.90016800	0.97696200
C	-2.60755600	-2.07532900	0.48888600
C	-1.55303100	-2.67107500	1.23228400
C	-0.60774100	-3.41904100	0.48862100
C	-1.44443400	-2.51416300	-1.66319900
C	-2.55484500	-1.99889500	-0.94029700
C	-0.55399500	-3.34091200	-0.93571100
C	-1.30559900	3.42586000	1.53791400
C	-0.91903200	2.60515200	2.66614300
C	-2.43060900	3.10590400	0.78899600
C	-1.67256300	1.50157500	3.00931200
C	-1.00877300	0.27284300	3.40717000
C	0.39738900	0.20467000	3.55021800
C	0.97833500	-1.07866400	3.40409900
C	-1.11323500	-2.02331600	2.47760300
C	-1.75246600	-0.82398700	2.87762100
C	0.23571300	-2.17554100	2.87732500
C	-1.19828200	3.58000100	-1.28086900
C	-0.03117800	3.91126900	-0.49403400
C	-2.37530100	3.18614700	-0.65839900
C	-0.08357100	3.83609700	0.88184900
C	1.04210900	3.28905800	1.61812600
C	2.24009100	2.91592300	0.96458700
C	3.02713500	1.93827900	1.61853900
C	1.19792000	1.38238800	3.19086300
C	0.52944700	2.53490600	2.71390700
C	2.51537600	1.18425800	2.71418800
C	-2.67246700	1.41071600	-2.33394300
C	-1.44546800	1.82925900	-2.97709000
C	-3.13140600	2.06867100	-1.19692800
C	-0.72466100	2.88525100	-2.46000700
C	0.72357100	2.81604300	-2.40610000
C	1.43106000	1.72010000	-2.95509300
C	2.70908800	1.46486700	-2.40428400

C	2.29590300	2.99603600	-0.50149900
C	1.14929100	3.44379800	-1.19883900
C	3.13405300	2.09227200	-1.19719000
C	0.66448700	0.59059700	-3.49969200
C	-0.74874000	0.64837000	-3.45492500
C	1.23793600	-0.70337700	-3.45112100
C	4.12571500	-0.03930900	-1.27844700
C	3.30716300	0.14295200	-2.45642400
C	2.59140600	-0.91695400	-2.97135400
C	4.18600500	-1.27798800	-0.65472500
C	4.01884100	-0.19402700	1.54096200
C	3.95057100	1.09203900	0.88382000
C	4.00281600	1.16734200	-0.49146900
C	4.13111700	-1.35738300	0.79228900
C	2.47991800	-2.46094500	2.23612100
C	2.36494700	-1.24389100	3.00734500
C	3.11411500	-0.13743700	2.66736200
C	3.34058800	-2.52004400	1.14755200
C	1.63352100	-3.70856400	-0.15798200
C	0.74144500	-3.63773200	0.97661500
C	1.15347000	-3.02706100	2.14317800
C	2.90763600	-3.15949500	-0.07948300
C	2.65344400	-2.21144500	-2.33067400
C	1.32566100	-2.77823400	-2.40052600
C	0.82908600	-3.51018600	-1.34190400
C	3.42955200	-2.39213700	-1.19311600
N	-7.83543100	-2.32640800	-0.00326200
H	-8.04057700	-2.72212500	-0.92071000
H	-7.89027400	-3.08226000	0.67930800
H	-8.57404400	-1.65815400	0.21666500
B	-6.36210300	-1.60293400	0.02173500
H	-6.41540400	-0.72946000	-0.81592200
H	-6.22983400	-1.17560300	1.14762300
H	-5.56516000	-2.47697900	-0.25371300
Li	-1.49109700	-0.10593200	-0.10730900

Li@C₇₀⁶⁻ts1

11			
C	2.99122100	0.48267000	-2.30710400
C	2.61687700	-0.92726600	-2.34256800
C	3.59616100	0.99009800	-1.15583300
C	2.89012500	-1.76095000	-1.28795300
C	1.90069400	-2.73072200	-0.87158900
C	0.70803000	-2.94159500	-1.60565100
C	-0.38378800	-3.48729100	-0.88816100
C	2.13888000	2.98153400	-1.29493200
C	1.51675200	2.44152000	-2.47125300
C	3.16463100	2.28126800	-0.64306600
C	1.92762700	1.20752000	-2.95315800
C	0.93514000	0.25873900	-3.43083700
C	-0.43834400	0.59434900	-3.50189300
C	-1.34618300	-0.49017700	-3.45223300
C	0.42768000	-2.06667000	-2.74655700

C	1.35818200	-1.04814800	-3.05599700
C	-0.92141600	-1.79887500	-3.08166900
C	2.16535900	2.84129400	1.53790000
C	1.11073100	3.56432100	0.85441900
C	3.17875200	2.20924900	0.80224700
C	1.09812200	3.63252700	-0.52420100
C	-0.15659700	3.50730500	-1.24413300
C	-1.39100700	3.39952800	-0.55894700
C	-2.43535900	2.75033700	-1.25761300
C	-0.87366800	1.90020200	-2.98333700
C	0.09883400	2.76906900	-2.43631700
C	-2.17974700	2.01104900	-2.44820100
C	3.03138100	0.25369300	2.28109600
C	1.97987700	0.90980700	3.01311900
C	3.61878700	0.87421800	1.17713800
C	1.56245400	2.18560800	2.66408600
C	0.14446500	2.51317600	2.68776100
C	-0.81879900	1.59281800	3.16280600
C	-2.13402600	1.75515600	2.66504700
C	-1.37792800	3.32619300	0.91000200
C	-0.13152400	3.36699600	1.58103800
C	-2.41033300	2.60985200	1.55895800
C	3.68289700	-1.30628200	-0.10132400
C	2.90870600	-1.87677700	1.04570600
C	3.94226800	0.12553500	-0.03327000
C	2.65644100	-1.15411900	2.18318100
C	1.41096500	-1.34665300	2.90325900
C	0.47433800	-2.33050100	2.51059900
C	-0.86838200	-2.09815200	2.89378900
C	-0.37593700	0.24186100	3.54082000
C	0.99534600	-0.08332800	3.41239500
C	-1.28569600	-0.83311100	3.40036200
C	0.73393700	-3.08755400	1.28377400
C	1.91316400	-2.80175700	0.55258400
C	-0.37106800	-3.55971800	0.53418700
C	-3.09686200	-1.76555700	2.22391500
C	-1.97665500	-2.67702500	2.15814200
C	-1.73318200	-3.39333000	1.00466300
C	-3.92832800	-1.60033700	1.12438700
C	-3.94641300	0.82838700	1.48574100
C	-3.07321300	0.64808100	2.62266200
C	-2.65984100	-0.61634500	2.98432200
C	-4.36505700	-0.27096500	0.74559200
C	-3.97166900	0.96922900	-1.33523900
C	-3.53440500	2.10574500	-0.55814700
C	-3.52211900	2.03710600	0.81802300
C	-4.37854400	-0.19878400	-0.70127300
C	-3.13769100	-1.53700300	-2.34364100
C	-2.71262800	-0.31715200	-2.99261900
C	-3.11930300	0.90453400	-2.50031400
C	-3.94950900	-1.48348100	-1.21831500
C	-2.59868000	-3.23094800	-0.14309000
C	-1.75378500	-3.27581600	-1.31581200
C	-2.01697300	-2.44897800	-2.38820400
C	-3.67115600	-2.35164200	-0.08965200

N	6.75219100	-0.88485100	-0.17536300
H	7.13463200	-0.85270200	-1.12232000
H	7.50083300	-0.63243300	0.47335400
H	6.02194500	-0.14553600	-0.10158600
B	6.11651100	-2.29279500	0.18558100
H	4.83348900	-2.06082700	-0.15805700
H	6.45676900	-3.15778900	-0.56012100
H	6.05639000	-2.44707500	1.36771500
Li	1.71667700	0.63764400	0.01431200

$Li@C_{70}^{6-}ts2$

1 1

C	-2.86293000	-0.98416400	2.32463500
C	-2.07693800	-2.21240600	2.12677400
C	-3.61677300	-0.50652200	1.24901600
C	-2.13436400	-2.89845400	0.94472600
C	-0.91665300	-3.42090900	0.38605800
C	0.32150100	-3.37880500	1.08353600
C	1.49191800	-3.44423400	0.29270400
C	-2.87336900	1.80390100	1.76517400
C	-2.06991200	1.29908500	2.83939500
C	-3.63291500	0.91639800	0.97826700
C	-2.05612000	-0.08300200	3.09561100
C	-0.79390700	-0.74165300	3.40269100
C	0.41832800	-0.01599900	3.54227100
C	1.61078400	-0.74441300	3.32690700
C	0.37451800	-2.65910400	2.35182200
C	-0.81313500	-2.03826500	2.80916800
C	1.58884100	-2.04613900	2.73915700
C	-2.97949100	2.11950100	-1.08290800
C	-2.15864500	3.00037900	-0.27191600
C	-3.71270700	1.08011700	-0.45653000
C	-2.10460500	2.85148400	1.10196500
C	-0.83966500	2.99549900	1.79436000
C	0.34373100	3.38898700	1.11300400
C	1.56235300	2.98954900	1.70273400
C	0.41088000	1.42702500	3.24905200
C	-0.80835600	2.03270800	2.84784300
C	1.59456500	2.01969300	2.75129000
C	-3.02827300	-0.47681300	-2.22390800
C	-2.27400900	0.57299100	-2.82367400
C	-3.68255500	-0.25265900	-1.02033400
C	-2.26129100	1.85980100	-2.27694900
C	-1.00236500	2.59832100	-2.23569100
C	0.17219900	2.10407000	-2.84746900
C	1.39770200	2.58413000	-2.32657400
C	0.28478300	3.55326300	-0.34554100
C	-0.94687800	3.31460800	-1.00731700
C	1.45465800	3.30036600	-1.09532500
C	-3.16681800	-2.62740200	-0.15809500
C	-2.22649100	-2.64691600	-1.37224100
C	-3.85439300	-1.25409000	0.02042700
C	-2.24639500	-1.71256300	-2.36668000

C	-1.03998600	-1.38380800	-3.09232300
C	0.17201600	-2.07967000	-2.87411100
C	1.35802100	-1.38564600	-3.20569200
C	0.14554800	0.75976800	-3.44775100
C	-1.05430500	0.01144000	-3.37619900
C	1.34439700	0.01267700	-3.49074600
C	0.21032100	-3.05971000	-1.79275600
C	-0.97181400	-3.26485300	-1.03163700
C	1.43644200	-3.28585000	-1.12465400
C	3.40487300	-0.49272900	-2.47319700
C	2.62010600	-1.70413100	-2.56744400
C	2.66040700	-2.63741600	-1.55177900
C	4.19507400	-0.25849400	-1.35708400
C	3.45867800	2.08329700	-1.30991800
C	2.63089900	1.82821100	-2.46602800
C	2.60335900	0.57237400	-3.03381800
C	4.22516900	1.06210000	-0.75902900
C	3.56693000	1.77236900	1.49597700
C	2.77462200	2.83135300	0.91549400
C	2.72004300	2.98135700	-0.45357700
C	4.27995300	0.90184700	0.67817600
C	3.58185300	-0.99818700	2.06922100
C	2.83423700	-0.08794100	2.90774400
C	2.82749700	1.26274600	2.62655900
C	4.28473200	-0.51709600	0.97257900
C	3.48511200	-2.39932300	-0.38637900
C	2.74792400	-2.89122500	0.75746200
C	2.79734100	-2.20743900	1.95609300
C	4.23546400	-1.23767300	-0.28623400
Li	-1.39525600	0.30095300	0.99867700
H	-3.88499300	-3.45551800	-0.21678200
N	-6.47026600	-0.37030200	-0.03573100
H	-5.44697300	-0.95822400	0.01423500
H	-7.04302300	-0.92807900	-0.67330300
H	-6.87378400	-0.42189500	0.90145200
B	-6.24963200	1.04368900	-0.53668300
H	-6.30628900	1.91173900	0.26459800
H	-6.24946900	1.18851500	-1.71100800

$Li@C_{70}^{6-}1$

11

C	2.77487000	1.57669700	2.18454600
C	1.88743500	2.68106500	1.79047700
C	3.56600900	0.98300600	1.17830300
C	1.89132000	3.18541100	0.51499900
C	0.64844300	3.53053500	-0.11502000
C	-0.59031000	3.50110600	0.58269500
C	-1.75214300	3.36050800	-0.20919600
C	2.98138700	-1.25040000	1.98457700
C	2.12318500	-0.66032100	2.97790400
C	3.70425700	-0.45483900	1.10724900
C	2.02079500	0.73674000	3.06739300
C	0.70146700	1.32684400	3.27006000

C	-0.45266500	0.53269700	3.50277300
C	-1.69525000	1.12842400	3.18373300
C	-0.59945200	2.97101300	1.94266900
C	0.62725700	2.51756100	2.49022600
C	-1.76817900	2.33069300	2.41593800
C	3.12674200	-1.97182300	-0.75480500
C	2.38376000	-2.79878500	0.16227400
C	4.00811300	-0.85918200	-0.30228100
C	2.30250300	-2.46309200	1.49610900
C	1.05616300	-2.59706400	2.20326400
C	-0.09227800	-3.17775900	1.59158600
C	-1.34074300	-2.78915800	2.11578700
C	-0.33220200	-0.93012800	3.41632300
C	0.93654100	-1.48458000	3.09451300
C	-1.45843100	-1.67972900	3.01346900
C	3.02791000	0.42230400	-2.29034100
C	2.36104800	-0.74097700	-2.71070200
C	3.70077800	0.42305200	-1.04496900
C	2.42400700	-1.93885700	-1.94735700
C	1.21924800	-2.77357600	-1.82398400
C	0.02510300	-2.46509400	-2.50430300
C	-1.16751900	-2.96014300	-1.92551900
C	-0.00837400	-3.55189500	0.17435000
C	1.20532000	-3.31846400	-0.51722900
C	-1.18572200	-3.49597400	-0.60494800
C	2.94045200	2.81711400	-0.53873300
C	2.02871500	2.61944300	-1.75093400
C	3.60049300	1.50251100	-0.16881400
C	2.14155700	1.55387800	-2.59644300
C	0.96859100	1.03676000	-3.26420700
C	-0.29628500	1.66334100	-3.14897000
C	-1.41987800	0.83772900	-3.37132600
C	-0.04112200	-1.21812000	-3.29375000
C	1.09806800	-0.37588300	-3.33528300
C	-1.29197000	-0.58441600	-3.44550000
C	-0.42384000	2.78474100	-2.22226500
C	0.72987400	3.18636300	-1.49930600
C	-1.67069600	3.00554700	-1.59048300
C	-3.39828000	-0.09917800	-2.51455200
C	-2.70932100	1.14325800	-2.78515600
C	-2.83432900	2.20893200	-1.91680600
C	-4.18274400	-0.22953500	-1.37688900
C	-3.27238500	-2.47697200	-0.99191400
C	-2.45231100	-2.32793900	-2.17145200
C	-2.51147000	-1.16819800	-2.91323800
C	-4.11956900	-1.44770100	-0.59489900
C	-3.43008000	-1.77060600	1.73791200
C	-2.55367300	-2.83994700	1.31713600
C	-2.47779000	-3.18369200	-0.01543000
C	-4.20093100	-1.08698800	0.80444700
C	-3.66570100	1.04387100	1.90490700
C	-2.85911700	0.32514000	2.86649700
C	-2.74436700	-1.04733300	2.78274700
C	-4.31707600	0.35684000	0.89004200
C	-3.65211100	2.07921300	-0.72790300

C	-2.96838200	2.78690800	0.33161100
C	-2.97601700	2.28131900	1.61643200
C	-4.31130500	0.88916600	-0.45951700
Li	1.39361400	0.30505500	1.01285400
H	3.65629200	3.63628200	-0.69840700
N	6.57548900	-0.14410500	-0.01132600
H	7.54463300	-0.36318300	-0.25159000
H	6.53554400	-0.01274500	1.00177200
H	6.34525400	0.75186300	-0.44983100
B	5.62094000	-1.35718400	-0.52789000
H	5.83048600	-1.49407900	-1.70136100
H	5.84946800	-2.30693500	0.16841800

Li@C₇₀⁶⁻⁶

1 1

C	3.22169800	-0.46622100	-2.26990600
C	2.49841200	-1.74684800	-2.34262700
C	3.95581600	-0.12681800	-1.15695200
C	2.53174000	-2.60440200	-1.28322000
C	1.32116400	-3.25973500	-0.87101900
C	0.11132800	-3.15329300	-1.60619700
C	-1.08249800	-3.39107100	-0.88786300
C	3.09992800	2.19405300	-1.29956800
C	2.34463700	1.82692400	-2.46605700
C	3.86305200	1.21012400	-0.64261600
C	2.39232400	0.51301900	-2.92548900
C	1.19330200	-0.13428800	-3.41006500
C	-0.04311800	0.55641500	-3.49209500
C	-1.20943100	-0.24164100	-3.45148000
C	0.07777100	-2.23953000	-2.74407200
C	1.25522600	-1.51150900	-3.04317300
C	-1.14858000	-1.61788400	-3.07852200
C	3.07690500	2.03323300	1.54236700
C	2.25465800	3.01359300	0.85965800
C	3.85397800	1.13464300	0.80134600
C	2.27378900	3.10972300	-0.52571300
C	1.01984100	3.30998200	-1.23925300
C	-0.20874300	3.52836200	-0.54982900
C	-1.38707000	3.17659100	-1.24704100
C	-0.11304300	1.93099500	-2.97322900
C	1.06380800	2.51789500	-2.43103200
C	-1.34004400	2.39149400	-2.44134900
C	3.20726200	-0.69542600	2.24167600
C	2.37313300	0.21249700	2.98960700
C	3.94923000	-0.24901900	1.17826200
C	2.32077200	1.55670400	2.66068100
C	1.04335500	2.24772800	2.68806000
C	-0.13152300	1.61662800	3.16245800
C	-1.35612900	2.12911600	2.67066000
C	-0.21319700	3.45094100	0.91859300
C	1.00437000	3.15150800	1.58446300
C	-1.39781400	3.03309200	1.56800500
C	3.49511800	-2.47754700	-0.11028500

C	2.52606400	-2.72495800	1.03878300
C	4.29051900	-1.11069700	-0.03645000
C	2.48131300	-1.97469100	2.17424200
C	1.23377300	-1.81147100	2.88837300
C	0.06012400	-2.50631200	2.51039300
C	-1.16848300	-1.92254900	2.89941500
C	-0.06539100	0.19722300	3.53889300
C	1.17060300	-0.48119400	3.39465700
C	-1.23071000	-0.59233200	3.40827700
C	0.10145100	-3.29948600	1.28601900
C	1.31645600	-3.33168800	0.55251300
C	-1.08668300	-3.46072400	0.53759000
C	-3.22709300	-1.00289300	2.23126900
C	-2.39224500	-2.18134100	2.16442900
C	-2.35267300	-2.93517400	1.00981300
C	-3.98441300	-0.62001900	1.13272400
C	-3.35238100	1.72449600	1.49660200
C	-2.55874800	1.31639800	2.63209700
C	-2.49448800	-0.01337300	2.98977800
C	-4.05001600	0.77828800	0.75419600
C	-3.34114500	1.86962700	-1.32679000
C	-2.61720500	2.84787800	-0.54899000
C	-2.62092200	2.77606200	0.82866300
C	-4.04558900	0.85217700	-0.69144700
C	-3.21140000	-0.77019000	-2.33730100
C	-2.47544100	0.29142700	-2.98598600
C	-2.54120100	1.57894800	-2.49305600
C	-3.97567300	-0.49958400	-1.20992000
C	-3.14424100	-2.54544900	-0.13681200
C	-2.34458400	-2.81820400	-1.31183900
C	-2.37747100	-1.95029900	-2.38414000
C	-3.94184300	-1.41173100	-0.08224700
Li	1.29924200	1.14893000	-0.53439000
H	4.23252000	-3.28771300	-0.15323500
H	5.35964100	-1.34823200	-0.04917500

$Li@C_{70}^{6-5}ts$

11			
C	2.49435000	1.97090100	2.28033000
C	1.23879200	2.09370800	2.98206700
C	2.75971600	2.76330300	1.16975800
C	0.29150900	2.99092500	2.54456100
C	-1.11386900	2.61556400	2.53602400
C	-1.55358800	1.37684600	3.06314500
C	-2.77335700	0.87808000	2.54659500
C	3.70707700	0.80915700	0.03514600
C	3.47230400	0.01160200	1.20508300
C	3.37137400	2.16358700	0.01185800
C	2.85043100	0.57424400	2.28835700
C	1.81223100	-0.15477700	3.02437100
C	1.45646100	-1.47807900	2.65747600
C	0.15617800	-1.89419600	3.02619400
C	-0.54623400	0.41849700	3.53557900

C	0.83250200	0.77211400	3.43685700
C	-0.83700300	-0.95407600	3.46149000
C	2.52634600	1.93898300	-2.27404100
C	2.88272700	0.54104600	-2.24892800
C	2.77338000	2.75023700	-1.17386500
C	3.43830800	-0.01708100	-1.11713900
C	3.18084600	-1.39464600	-0.71124200
C	2.14257800	-2.12156900	-1.40011600
C	1.43163100	-3.11569700	-0.69095300
C	2.09784400	-2.09598700	1.50428700
C	3.28062200	-1.44688000	0.82650200
C	1.39490000	-3.04679800	0.78180800
C	0.57190200	3.79919400	-1.44178200
C	0.32367100	2.95906100	-2.58635300
C	1.77293800	3.69840500	-0.74490500
C	1.27967700	2.04916000	-2.99545300
C	0.87655200	0.72587900	-3.42627100
C	-0.49088200	0.35923800	-3.52854900
C	-0.78285300	-1.02028300	-3.43561700
C	1.50730700	-1.52523200	-2.58821000
C	1.85240200	-0.19569700	-2.95263900
C	0.20467900	-1.95589400	-2.96950500
C	0.55593900	3.81530200	1.38412600
C	-0.68694900	3.91594800	0.65318800
C	1.76213200	3.70954900	0.70775200
C	-0.67941300	3.90837300	-0.72477400
C	-1.69498900	3.16046200	-1.44527100
C	-2.76044600	2.51477200	-0.77118000
C	-3.35409500	1.42027000	-1.44260000
C	-1.50965000	1.32521300	-3.09479800
C	-1.07828700	2.57503700	-2.58675800
C	-2.73503000	0.83095400	-2.58518600
C	-2.76986300	2.52669500	0.69799000
C	-1.71046000	3.18025000	1.37605200
C	-3.37037200	1.44398600	1.37952100
C	-3.85640700	-0.88035300	-1.42799500
C	-4.04027100	0.36770100	-0.71688700
C	-4.04780800	0.37975200	0.66152600
C	-3.68430400	-2.06981300	-0.72707500
C	-1.89391400	-2.73695800	-2.27358200
C	-2.07667000	-1.49548300	-2.99534000
C	-3.03612100	-0.58828400	-2.57790400
C	-2.68165600	-3.01823700	-1.15815400
C	-0.69269800	-3.84407600	0.04242400
C	0.12934400	-3.56646000	-1.12659000
C	-0.47373900	-3.02377600	-2.26491700
C	-2.06063300	-3.58036900	0.02801700
C	-1.93482000	-2.68818600	2.31499300
C	-0.51239600	-2.95280000	2.32088600
C	0.09304200	-3.51295600	1.20863300
C	-2.69565800	-2.99332400	1.19397700
C	-3.87655100	-0.85423800	1.39887800
C	-3.07572200	-0.53920300	2.56276100
C	-2.12979900	-1.43715900	3.01375400
C	-3.69629800	-2.05420900	0.72596200

N	5.49059200	-2.81445900	-0.68387200
H	4.52279400	-2.22307200	-0.92679800
H	6.24355100	-2.30504400	-1.15033600
H	5.37406800	-3.72461700	-1.13355000
B	5.61356900	-2.87372800	0.82553400
H	6.30753700	-2.05441300	1.33040800
H	4.22411100	-2.04240800	1.15604300
H	5.21432500	-3.86163100	1.34804400
Li	-0.01390500	-1.40208800	-0.75482300

$Li@C_{70}^{6-5}ts2$

1 1

C	-3.12141000	-2.02805300	0.53472600
C	-2.47118000	-2.60042000	-0.62225300
C	-3.72920300	-0.77778100	0.42837400
C	-2.47376000	-1.91760500	-1.81787900
C	-1.30567200	-1.90513000	-2.65663000
C	-0.14348100	-2.64139700	-2.31146000
C	1.07737300	-2.16336200	-2.83307400
C	-2.78341500	-0.11902500	2.60802000
C	-2.11775000	-1.40632200	2.68521700
C	-3.56683400	0.20128100	1.48049500
C	-2.27885200	-2.33146300	1.66708400
C	-1.14998200	-3.12349800	1.21734300
C	0.11888400	-3.02620000	1.84353300
C	1.23602500	-3.36587400	1.04623500
C	-0.12345200	-3.35641000	-1.02778200
C	-1.26691400	-3.28681700	-0.19352400
C	1.11709300	-3.52816400	-0.36684000
C	-2.60431400	2.42558400	1.37608300
C	-1.76567100	2.09450800	2.50776300
C	-3.51132200	1.50561700	0.88423700
C	-1.87411400	0.85744400	3.14495400
C	-0.65331900	0.17468800	3.56372200
C	0.62176900	0.80092500	3.45826000
C	1.73742700	-0.06715300	3.36459700
C	0.29896400	-2.03614400	2.91471900
C	-0.81068300	-1.22220900	3.28469900
C	1.57716400	-1.46566000	3.10069100
C	-2.86305900	2.14331200	-1.43602000
C	-1.92411000	3.05200700	-0.87180900
C	-3.91903300	1.45034400	-0.59529100
C	-1.81188400	3.27911200	0.49248200
C	-0.50791600	3.42440700	1.07625700
C	0.67907200	3.54751400	0.29551100
C	1.88750500	3.18074800	0.92088600
C	0.71221300	2.12793000	2.82702900
C	-0.47927200	2.71972000	2.32443500
C	1.91257100	2.48730800	2.17583400
C	-3.13687900	-0.62977300	-1.92582500
C	-2.38475900	0.16654900	-2.84955900
C	-3.87300500	-0.09250400	-0.85434500
C	-2.21109900	1.51879200	-2.50552200

C	-0.88921100	2.13101600	-2.71267200
C	0.19964700	1.41153000	-3.24821100
C	1.48553300	1.89058100	-2.90275500
C	0.55943700	3.37482000	-1.15406400
C	-0.71569800	3.09216400	-1.69671800
C	1.66277500	2.85655200	-1.86993300
C	0.03055600	-0.02170800	-3.52957800
C	-1.23249600	-0.60849500	-3.25574300
C	1.15756200	-0.86351500	-3.42390500
C	3.55036900	1.45161900	-1.86368700
C	2.64427700	1.01520400	-2.90199200
C	2.48219700	-0.33001300	-3.15534600
C	4.25785500	0.51907800	-1.11570600
C	3.77889400	1.77925500	0.93407600
C	3.04006100	2.74367800	0.15085200
C	2.92981200	2.58394100	-1.21449700
C	4.37577800	0.68728200	0.31810400
C	3.60624600	-0.77782000	2.13425200
C	2.98430900	0.36257000	2.76758100
C	3.06300400	1.61062700	2.17977700
C	4.28824100	-0.62742900	0.93213900
C	3.26728300	-2.68862000	0.07582900
C	2.55841800	-2.83665300	1.32473300
C	2.72565900	-1.90484500	2.33048400
C	4.11605600	-1.60385900	-0.11854900
C	3.22440500	-1.30622300	-2.38903200
C	2.34000400	-2.43187500	-2.17403200
C	2.36710100	-3.11057700	-0.97319700
C	4.09155400	-0.89589200	-1.38674000
Li	-0.91136300	0.17198900	1.32957700
N	-6.59513700	-0.53161800	-0.93212300
H	-5.46977600	-0.31344500	-1.07569900
H	-7.08185000	0.33190100	-1.18680500
H	-6.81701000	-1.26427800	-1.61134100
B	-6.72851100	-0.93609900	0.51857100
H	-6.64161400	-2.08710500	0.76743800
H	-6.89786900	-0.05872200	1.29279800
H	-4.92934700	1.86220600	-0.74415200

$Li@C_{70}^{6-5}$

11			
C	-3.12523200	-2.34277000	0.71651300
C	-2.37587700	-2.99626700	-0.36934600
C	-3.90578000	-1.23588300	0.47241100
C	-2.44640900	-2.49218400	-1.63792300
C	-1.23871000	-2.42843900	-2.43766000
C	-0.00579200	-2.97093100	-1.98973800
C	1.16069000	-2.39809200	-2.53814000
C	-3.05047800	-0.21693700	2.54044300
C	-2.26413700	-1.38688500	2.79740000
C	-3.84998100	-0.13578800	1.38631300
C	-2.28922100	-2.41856100	1.88061800
C	-1.05981200	-3.11836000	1.53832900

C	0.16392400	-2.80844500	2.17759100
C	1.33746600	-3.11112500	1.44703300
C	0.05866900	-3.52078500	-0.63250800
C	-1.11532600	-3.47518200	0.16273400
C	1.28640400	-3.46139400	0.06489100
C	-3.15315800	2.16126500	1.05948600
C	-2.31681400	2.07405900	2.22421600
C	-3.91853100	1.08961600	0.64766800
C	-2.27408000	0.91356600	2.96900300
C	-1.01006300	0.43991800	3.49944500
C	0.17825300	1.19478500	3.35629900
C	1.38814900	0.46413600	3.38361300
C	0.19458900	-1.69110900	3.13444900
C	-1.00177200	-0.98089100	3.39004900
C	1.39587200	-0.95769000	3.27356200
C	-3.28961800	1.53804800	-1.70076900
C	-2.49449200	2.68276700	-1.25932100
C	-4.29970700	0.83619300	-0.81520200
C	-2.41253300	2.98111800	0.08414000
C	-1.15676300	3.39004700	0.68024100
C	0.01862400	3.56753500	-0.09943500
C	1.24985100	3.41628500	0.58240900
C	0.13365000	2.43981300	2.57470200
C	-1.09400000	2.82789300	1.99019100
C	1.30493500	2.86086200	1.89470200
C	-3.25974700	-1.30976200	-1.90986500
C	-2.54887500	-0.53909400	-2.79388400
C	-4.28229300	-0.76783600	-0.93700200
C	-2.55815100	0.90098300	-2.68135000
C	-1.31054700	1.63463600	-2.94394000
C	-0.12178900	0.98092100	-3.36043200
C	1.08933400	1.64184700	-3.06250900
C	-0.04124300	3.22671800	-1.52345100
C	-1.27614400	2.74557200	-2.05643800
C	1.12986600	2.74502000	-2.14765000
C	-0.11454800	-0.49526500	-3.47509800
C	-1.28974400	-1.20856800	-3.15162500
C	1.10623200	-1.17447900	-3.27466900
C	3.16220600	1.57778300	-1.95921400
C	2.34185700	0.91923100	-2.94842300
C	2.34768200	-0.45704500	-3.04747500
C	3.95508500	0.82667300	-1.09865800
C	3.28576500	2.25192800	0.78575800
C	2.46147700	3.02818300	-0.11501900
C	2.40446300	2.69950600	-1.45417600
C	4.01662700	1.17310000	0.30644000
C	3.36451800	-0.15706500	2.26528700
C	2.59293000	0.96743500	2.74868000
C	2.56009800	2.14390600	2.03080400
C	4.05788000	-0.06310600	1.06785700
C	3.30844000	-2.31464100	0.44131800
C	2.58196300	-2.40191400	1.68775300
C	2.60786300	-1.34905800	2.57681700
C	4.03209400	-1.17099900	0.13155100
C	3.17995100	-1.24503400	-2.16913300

C	2.43423200	-2.43905200	-1.83961000
C	2.49566600	-2.96190600	-0.56556600
C	3.96350700	-0.61939000	-1.20684500
H	-5.28979600	-1.10249500	-1.20771900
H	-5.31516900	1.18894700	-1.02452900
Li	-1.26390500	0.93234900	-0.79320100

Li@C₃₆

1 1			
C	0.71728500	-2.13245900	-1.25591700
C	1.41348300	-1.14609100	-2.02548000
C	0.71812400	0.02127700	-2.47316100
C	1.41549700	1.18100200	-2.00375300
C	0.72045300	2.15420600	-1.21811400
C	1.41804800	2.32739100	0.02127200
C	0.72046800	2.13161800	1.25565700
C	1.41580700	1.14456800	2.02555400
C	0.71846900	-0.02308600	2.47200900
C	1.41432100	-1.18278700	2.00322000
C	0.71802200	-2.15610000	1.21741500
C	1.41460500	-2.32818400	-0.02135600
C	-0.72861800	-2.13242200	-1.25650300
C	-1.42202300	-2.26637700	-0.01945100
C	-0.72871400	-2.15567100	1.21863200
C	-1.42063800	-1.15033600	1.95325800
C	-0.72736100	-0.02223300	2.47478200
C	-1.41889400	1.11745200	1.97379600
C	-0.72587100	2.13276300	1.25641100
C	-1.41923300	2.26791900	0.01989800
C	-0.72613100	2.15533500	-1.21835600
C	-1.41979200	1.15163600	-1.95326900
C	-0.72756100	0.02247500	-2.47450800
C	-1.42067200	-1.11622200	-1.97329300
C	-2.64376500	-0.68859500	-1.21940900
C	-2.64500100	-1.39958100	-0.01222000
C	-2.64409500	-0.70960600	1.20730500
C	-2.64256200	0.69147600	1.21980000
C	-2.64289900	1.40229000	0.01273100
C	-2.64323200	0.71229600	-1.20701700
C	2.58760600	-0.69833800	-1.23322700
C	2.58868300	0.71793300	-1.22009600
C	2.59002100	1.41538200	0.01325200
C	2.58876500	0.69589000	1.23334100
C	2.58791400	-0.72063800	1.21971400
C	2.58827600	-1.41749900	-0.01351900
Li	0.82242200	0.00663200	0.00120200

Li@C₃₆^{AB}

1 1			
C	-0.82560000	1.18380800	-2.29557000
C	-1.16578900	2.28042600	-1.43100900
C	-2.06862600	2.06444400	-0.34360100

C	-1.42839000	2.46791100	0.87316800
C	-1.30830200	1.52822800	1.95189900
C	0.06927900	1.40629700	2.30335100
C	0.69224500	0.11074500	2.29416200
C	1.82278900	0.15890300	1.42757500
C	1.93242900	-0.76885200	0.34280100
C	2.08104800	-0.02685900	-0.86910700
C	1.17453100	-0.23421500	-1.94979100
C	0.59158500	1.03090600	-2.30018400
C	-1.66108700	0.00368200	-2.29558600
C	-1.04763500	-1.27849600	-2.25045500
C	0.33932700	-1.41296300	-1.95266500
C	0.41142000	-2.30983100	-0.85014200
C	1.09832600	-1.94666800	0.34330300
C	0.15707600	-2.12821600	1.39680600
C	-0.14321900	-1.06871100	2.29633200
C	-1.56020800	-0.91413200	2.25368400
C	-2.14338300	0.34715100	1.95197600
C	-3.02491900	0.11982300	0.85448300
C	-2.90274100	0.88289200	-0.34290700
C	-2.76887100	-0.06168200	-1.39904500
C	-2.91111500	-1.45001400	-0.86099100
C	-1.85195800	-2.20215800	-1.38587300
C	-0.95125500	-2.84161200	-0.52392000
C	-1.10914000	-2.72877600	0.86370200
C	-2.16765900	-1.97704100	1.39040300
C	-3.07015600	-1.33711700	0.52845700
C	0.09392400	2.82688900	-0.87203700
C	-0.06670900	2.94067400	0.53155200
C	0.84774900	2.29380600	1.40174200
C	1.91760200	1.53776000	0.86979400
C	2.07655400	1.42422800	-0.53045200
C	1.16706200	2.06668100	-1.40064200
Li	-0.02860200	0.72891100	0.00372800
B	4.99403100	-0.70222400	-0.05929100
H	4.74135500	-0.55738400	-1.23702500
H	4.71407400	0.27023900	0.60916100
H	4.54166300	-1.73399200	0.39099900
N	6.62354200	-0.84832200	0.03330800
H	7.09082000	-0.01698400	-0.32927600
H	6.93093500	-0.97851700	0.99738300
H	6.95490900	-1.64820000	-0.50639200

$Li@C_{36}^{6-6}ts1$

11			
C	0.61073700	0.68948800	-2.25615600
C	-0.59084800	1.43113400	-2.30544200
C	-1.85621800	0.79347000	-1.99219000
C	-2.47207000	1.51635700	-0.94028000
C	-2.86513800	0.84319400	0.26544000
C	-2.22432800	1.50323000	1.37116500
C	-1.40173400	0.76933300	2.25858200
C	-0.09540300	1.40541700	2.30453700

C	1.06630300	0.66630300	1.99075800
C	1.80708300	1.35010500	0.94527600
C	2.07555900	0.63706900	-0.26708200
C	1.54920400	1.35877400	-1.37485800
C	0.55521300	-0.75620600	-2.21875900
C	1.37955800	-1.48720700	-1.34047800
C	2.15270400	-0.84860600	-0.28170400
C	1.61564400	-1.50028500	0.91020000
C	0.99903400	-0.77966800	1.94923300
C	-0.25291300	-1.42924300	2.20913600
C	-1.47233100	-0.67022700	2.24706600
C	-2.33119000	-1.31732900	1.32889900
C	-2.94813100	-0.58992400	0.26577000
C	-2.56818600	-1.30497400	-0.91225500
C	-1.92305500	-0.64613300	-1.98440400
C	-0.72372400	-1.40468600	-2.21521100
C	-0.68803000	-2.62407200	-1.40300900
C	0.59088900	-2.65605900	-0.82579100
C	0.73808900	-2.66543100	0.56159300
C	-0.39078300	-2.64151800	1.39545200
C	-1.68350000	-2.57782500	0.81338200
C	-1.83077000	-2.57108900	-0.56207400
C	-0.43510800	2.60098400	-1.40620900
C	-1.57236300	2.64884600	-0.57225900
C	-1.42143600	2.64051500	0.83473700
C	-0.13296600	2.58419300	1.40811400
C	1.02184500	2.54251300	0.57588500
C	0.86783100	2.54946300	-0.83594600
N	5.16361500	0.54013900	0.00629000
H	4.48311900	1.09877800	0.53201400
H	5.19814500	0.90684800	-0.94764000
H	6.08303000	0.70574500	0.42522700
B	4.83527000	-1.03546500	0.05391000
H	3.63919300	-1.12124200	-0.44792800
H	5.55830400	-1.62609200	-0.69187800
H	4.71980100	-1.38149900	1.19558800
Li	-0.30001800	0.81812300	-0.00855600

$Li@C_{36}^{6-}ts2$

11			
C	0.91125100	0.42385400	-2.15844600
C	-0.07048700	1.40956100	-2.32462400
C	-1.49324900	1.08246700	-2.10938300
C	-1.99203500	1.94753300	-1.11963700
C	-2.65710900	1.42728900	0.05164900
C	-1.95138700	1.92537100	1.20952000
C	-1.41903700	1.04159500	2.16471500
C	0.01049700	1.36541100	2.33755200
C	0.98579300	0.38324000	2.11714700
C	1.95014000	0.87237000	1.12646200
C	2.31933400	0.07632900	-0.04756200
C	1.90910400	0.89449900	-1.19115100
C	0.53652500	-0.97184600	-2.08629200

C	1.10648400	-1.83923600	-1.17938500
C	2.08016300	-1.45896300	-0.05738700
C	1.14528100	-1.86055400	1.08932700
C	0.60797300	-1.01106700	2.03229500
C	-0.80999200	-1.38153300	2.19506400
C	-1.82654000	-0.33315500	2.12859700
C	-2.74502900	-0.76517200	1.15957500
C	-3.09751500	0.07190400	0.04643300
C	-2.78418300	-0.74363600	-1.09370100
C	-1.89947700	-0.29281000	-2.08538800
C	-0.88630100	-1.33939300	-2.20683500
C	-1.18506900	-2.48114900	-1.44437200
C	0.02440500	-2.74732600	-0.72655900
C	0.04831600	-2.76035500	0.65707200
C	-1.13533300	-2.50876400	1.42171500
C	-2.34421200	-2.13951700	0.69368500
C	-2.36780600	-2.12660300	-0.66813800
C	0.27505300	2.52541800	-1.42179300
C	-0.86522000	2.82533300	-0.68295000
C	-0.84050500	2.81151300	0.75172200
C	0.32475700	2.49776600	1.44527600
C	1.52492900	2.16444400	0.70174700
C	1.50020000	2.17862300	-0.72750600
N	5.05500000	0.16261500	-0.06232000
H	5.25108000	0.79240600	0.71756900
H	5.27965500	0.61459300	-0.94992400
B	5.48386100	-1.23398200	0.09842400
H	5.65092700	-1.87351000	-0.88467300
H	5.56303700	-1.65357800	1.20347900
Li	-0.21257900	0.67439300	0.00400700
H	3.02703900	-2.02423400	-0.07949800
H	3.72339500	0.17213100	-0.06551000

$Li@C_{36}^{6-61}$

1 1

C	0.39791800	0.18921000	-2.44324500
C	-0.02694600	1.49691500	-2.25338800
C	-1.36001100	1.78136000	-1.68569200
C	-1.15924000	2.61185700	-0.56710100
C	-1.70246800	2.25625600	0.72634500
C	-0.56383600	2.22201100	1.62477700
C	-0.26823700	1.06078700	2.35569100
C	1.13553200	0.72089800	2.06916800
C	1.50153700	-0.51274000	1.57083900
C	2.55106000	-0.39521500	0.45680400
C	1.88862500	-0.95776300	-0.81282900
C	1.68190100	0.03400700	-1.72446900
C	-0.52367600	-0.91942300	-2.33621000
C	-0.18065500	-2.06939200	-1.65929700
C	1.10976900	-2.27967700	-0.84468200
C	0.41116800	-2.45475300	0.50810000
C	0.55359500	-1.60161400	1.57814100
C	-0.79759800	-1.37042300	2.13778800

C	-1.23816900	0.00444100	2.40409700
C	-2.46295500	0.14740100	1.74729100
C	-2.66807300	1.21978300	0.80355000
C	-3.03926000	0.53232800	-0.40445000
C	-2.31714000	0.71567500	-1.58910000
C	-1.93925600	-0.63261200	-2.03706500
C	-2.50469100	-1.64065300	-1.25176600
C	-1.39860800	-2.50407500	-0.93050200
C	-1.03995600	-2.73609800	0.38018800
C	-1.76177200	-2.12209900	1.46423000
C	-2.83010400	-1.17914400	1.13815900
C	-3.17679700	-0.94739300	-0.15654200
C	0.98352100	2.24217400	-1.46246300
C	0.29621900	2.90984800	-0.43233000
C	0.66239400	2.67358400	0.90938100
C	1.70874600	1.77015900	1.20041800
C	2.44797900	1.12171400	0.18077600
C	2.04027700	1.35276100	-1.13870000
N	5.08482100	-0.69938400	-0.24707500
H	5.24084600	0.30914100	-0.31289800
H	5.98160100	-1.12678100	-0.00569500
B	3.98880200	-1.07916600	0.90037900
H	3.89731500	-2.28113100	0.90720600
H	4.39353100	-0.59884600	1.92494500
Li	-0.02885100	0.56845300	-0.03539700
H	1.73873000	-3.12169300	-1.15587100
H	4.83201600	-1.03510500	-1.17933300

$Li@C_{36}^{6-6}$

1 1

C	0.43285400	-2.63213500	0.00044200
C	1.16284800	-2.18779700	-1.16997700
C	0.54691600	-1.38949700	-2.15167900
C	1.39333200	-0.19498000	-2.35944500
C	0.85055300	1.08062800	-2.14606300
C	1.66711200	1.81535500	-1.17283100
C	1.10894000	2.64644800	-0.00033800
C	1.66693000	1.81576500	1.17249700
C	0.85013400	1.08138200	2.14577200
C	1.39283800	-0.19417000	2.35960000
C	0.54649500	-1.38876300	2.15212900
C	1.16265200	-2.18742700	1.17086700
C	-0.98408700	-2.53875300	0.00032200
C	-1.62314100	-1.91236500	1.12920500
C	-0.87833900	-1.24833300	2.11724000
C	-1.46574600	0.09116900	2.21066900
C	-0.57721200	1.26057900	2.05778500
C	-1.15622300	2.09458600	1.12299100
C	-0.45692600	2.86315700	-0.00051300
C	-1.15594600	2.09404100	-1.12367800
C	-0.57677900	1.25981000	-2.05824300
C	-1.46528900	0.09039900	-2.21080800

C	-0.87790900	-1.24912600	-2.11704000
C	-1.62286600	-1.91278100	-1.12884600
C	-2.73556300	-1.01109200	-0.68263300
C	-2.73582100	-1.01095300	0.68258700
C	-2.62891300	0.23149300	1.44146000
C	-2.40646300	1.43471000	0.69231500
C	-2.40631500	1.43443000	-0.69313100
C	-2.62868300	0.23101300	-1.44196000
C	2.38385400	-1.46719500	-0.72875600
C	2.54633400	-0.30824900	-1.46128500
C	2.66155000	0.96233800	-0.73114500
C	2.66146600	0.96259000	0.73127700
C	2.54612500	-0.30774700	1.46177800
C	2.38371800	-1.46691700	0.72959100
Li	0.53313000	-0.20709600	0.00013100
H	-0.67837300	3.93403700	-0.00080400
H	1.58441500	3.63757200	-0.00051200

$Li@C_{36}^{5-5}ts2$

11			
C	-2.32195500	-1.18398600	-1.24228100
C	-1.19579700	-1.67043900	-2.01414600
C	-0.24802400	-0.75030200	-2.50166000
C	1.04799000	-1.17308900	-1.97895700
C	1.83561800	-0.30421400	-1.22302700
C	2.39928300	-0.96845400	0.00009000
C	1.83558500	-0.30421100	1.22321400
C	1.04785100	-1.17308600	1.97904600
C	-0.24820800	-0.75031100	2.50166200
C	-1.19594100	-1.67044200	2.01406400
C	-2.32205700	-1.18399900	1.24212600
C	-2.32605000	-1.89724500	-0.00007800
C	-2.60170800	0.22296300	-1.24148300
C	-2.85195200	0.86709100	-0.00009200
C	-2.60181200	0.22294900	1.24131300
C	-1.76363900	1.12003900	2.01531700
C	-0.54529800	0.65859300	2.50875900
C	0.46749900	1.57517600	1.96473000
C	1.53339000	1.08961500	1.20723500
C	1.83137400	1.91558900	0.00014100
C	1.53341100	1.08960400	-1.20701000
C	0.46765000	1.57517700	-1.96465400
C	-0.54509700	0.65860300	-2.50877500
C	-1.76347100	1.12005400	-2.01542100
C	-1.53886100	2.38337500	-1.24903300
C	-2.16807200	2.18657000	-0.00006200
C	-1.53897200	2.38335500	1.24894400
C	-0.16148400	2.60662900	1.21464700
C	0.67764400	3.00523600	0.00002900
C	-0.16140800	2.60664500	-1.21462800
C	-0.50193800	-2.72234700	-1.22288900
C	0.87959000	-2.41842400	-1.21179400
C	1.60829300	-2.25981000	0.00006800

C	0.87950100	-2.41841400	1.21187400
C	-0.50202300	-2.72234500	1.22286300
C	-1.19987100	-2.85875100	-0.00003600
H	4.89313500	1.19534200	-0.81357900
H	4.89349000	1.19541600	0.81321000
N	4.35313300	0.90394300	-0.00005100
B	4.17484300	-0.66039800	0.00002100
H	4.55297300	-1.16091400	1.02661000
H	4.55291900	-1.16103100	-1.02655100
H	3.12399200	1.82713000	-0.00009700
Li	-0.27079000	-0.70588200	0.00000300
H	1.00344600	4.05174000	0.00007700

*Li@C*₃₆⁵⁻⁵1

1 1

C	-1.97680600	-1.70208300	-1.23782600
C	-0.75573800	-1.86318300	-1.99748500
C	-0.07752600	-0.72828500	-2.47658300
C	1.28637800	-0.80392600	-1.95535700
C	1.85131600	0.22522700	-1.22512900
C	2.60404900	-0.31217000	0.00031100
C	1.85095200	0.22534300	1.22541600
C	1.28581100	-0.80372300	1.95564300
C	-0.07824500	-0.72810000	2.47653200
C	-0.75629800	-1.86307700	1.99741100
C	-1.97722700	-1.70208400	1.23745200
C	-1.78874600	-2.39437400	-0.00014700
C	-2.62596600	-0.41790900	-1.22969200
C	-3.05274600	0.12867400	-0.00030000
C	-2.62647000	-0.41794800	1.22915600
C	-2.02956200	0.66949600	1.99143400
C	-0.72847000	0.55247500	2.47867900
C	0.00566300	1.71688900	1.95297000
C	1.22113300	1.53119800	1.20950100
C	1.12118300	2.26883400	0.00007200
C	1.22143800	1.53106600	-1.20950600
C	0.00632500	1.71662500	-1.95311000
C	-0.72765000	0.55231400	-2.47897400
C	-2.02881900	0.66939500	-1.99176400
C	-2.12993400	1.94277000	-1.23021800
C	-2.71829900	1.61142700	-0.00018900
C	-2.13051400	1.94283900	1.22980900
C	-0.86797900	2.55903500	1.23946600
C	-0.17475700	3.11524600	-0.00006400
C	-0.86768100	2.55889200	-1.23964100
C	0.18319500	-2.72120500	-1.21872200
C	1.43908900	-2.07775200	-1.20296700
C	2.10004200	-1.76753500	0.00029500
C	1.43872800	-2.07761000	1.20343200
C	0.18287800	-2.72112300	1.21893600
C	-0.45309400	-3.04171600	0.00002800
H	5.62708700	1.54017200	0.00054900
H	4.26089900	1.93304400	0.82577900

N	4.60950800	1.44004200	0.00027200
B	4.25263000	-0.15525200	0.00033600
Li	-0.14653200	-0.65016000	0.00062700
H	-0.02139400	4.20161900	-0.00012300
H	4.26137300	1.93283600	-0.82556200
H	4.71402600	-0.60239800	1.01638400
H	4.71397000	-0.60247200	-1.01570200

$Li@C_{36}^{5-5}$

1 1

C	-0.74697900	0.08707500	-2.50690600
C	-1.66131700	-0.92782700	-2.04519800
C	-1.14493700	-2.00619600	-1.25420600
C	-1.87420500	-2.06363700	0.00024700
C	-1.14497900	-2.00587400	1.25471500
C	-1.66140600	-0.92733300	2.04546400
C	-0.74705400	0.08774900	2.50684100
C	-1.19551800	1.35361600	2.02289500
C	-0.31635500	2.18370400	1.23769800
C	-0.97046300	2.50063100	-0.00031800
C	-0.31634300	2.18337200	-1.23832700
C	-1.19548000	1.35311800	-2.02327600
C	0.66408100	-0.18131900	-2.51673900
C	1.56323900	0.83893700	-1.96173400
C	1.08908200	1.91572800	-1.23428700
C	1.96498200	2.20280500	-0.00030200
C	1.08909200	1.91610000	1.23382300
C	1.56323100	0.83952500	1.96157500
C	0.66402800	-0.18065200	2.51678100
C	1.13974700	-1.39498200	2.02019400
C	0.26656300	-2.24522100	1.25178100
C	0.92411800	-2.47643600	0.00035700
C	0.26659900	-2.24556200	-1.25121600
C	1.13978400	-1.39557300	-2.01980900
C	2.40571700	-1.16190900	-1.25256800
C	2.61787100	0.20098500	-1.21678400
C	3.02103000	1.02202900	-0.00011200
C	2.61785300	0.20134700	1.21679600
C	2.40569300	-1.16153800	1.25291700
C	2.21825000	-1.80363100	0.00026900
C	-2.69815100	-0.26482500	-1.24329200
C	-2.82082200	-0.97139500	0.00011500
C	-2.69818200	-0.26455100	1.24335000
C	-2.42091900	1.12096800	1.23701400
C	-2.26216500	1.80660400	-0.00023000
C	-2.42090700	1.12066900	-1.23735200
H	2.39692000	3.20835500	-0.00045800
Li	-0.80419900	-0.03139600	-0.00014300
H	4.06699400	1.34684500	-0.00015500

$Li@C_{36}^{6-5}ts1$

1 1

C	-1.67593000	1.41168100	-1.80058700
C	-1.81997900	0.07970100	-2.28839400
C	-0.68447700	-0.77607400	-2.41940900
C	-0.99541300	-1.94753100	-1.67533300
C	-0.11670400	-2.41830300	-0.65459800
C	-0.91461800	-2.52942800	0.51575700
C	-0.53245600	-1.87747800	1.72007900
C	-1.65593200	-1.08597300	2.09900800
C	-1.51856400	0.30881900	2.33973400
C	-2.48253900	0.94085700	1.49654700
C	-2.08956100	1.94978600	0.56942800
C	-2.58125900	1.54038400	-0.70542100
C	-0.35246000	1.98558600	-1.70274300
C	0.02108700	2.70281200	-0.51756900
C	-0.76582600	2.52255300	0.67411600
C	0.09493800	2.08239800	1.72383200
C	-0.19811300	0.87465600	2.44470400
C	0.93787300	0.02111000	2.33177100
C	0.79216500	-1.30842300	1.81692900
C	1.70066600	-1.47283800	0.73226200
C	1.20733200	-1.84916400	-0.54595800
C	1.61376800	-0.85462700	-1.49935100
C	0.63827300	-0.21157600	-2.31753200
C	0.77123300	1.20588300	-2.12852400
C	1.87164800	1.43569200	-1.16673500
C	1.42801800	2.37187300	-0.19799200
C	1.46486200	1.96281400	1.16621300
C	1.99153700	0.71811500	1.55810900
C	2.51668800	-0.20403800	0.58364300
C	2.41998400	0.17694000	-0.80586700
C	-2.90322000	-0.62011700	-1.53530100
C	-2.39582200	-1.87070100	-1.15575400
C	-2.35187300	-2.23797200	0.19729600
C	-2.80438600	-1.34048700	1.17272800
C	-3.31401800	-0.08722700	0.80400400
C	-3.35336800	0.27529800	-0.55165000
H	6.24224400	-0.67358000	-1.19431100
H	6.06758800	0.52898300	-0.08276400
N	5.57707300	-0.23130400	-0.55672600
B	4.98338600	-1.31704800	0.47781300
H	5.79817800	-1.55793300	1.32093400
H	4.51433100	-2.22170000	-0.15897400
H	4.82844000	0.17640600	-1.13007400
H	4.01913200	-0.68632700	1.02304300
Li	0.26410900	0.46283600	0.02183400

$Li@C_{36}^{6-5}ts2$

1 1

C	-0.51945100	-2.25266500	-1.22502300
C	-0.81631900	-2.64681600	0.11756100
C	0.00190000	-2.16635700	1.19280800
C	-0.83115100	-1.50540700	2.14686600
C	-0.54720800	-0.15260400	2.51217800

C	-1.71368100	0.64683300	2.28670200
C	-1.61289600	1.79586200	1.44731300
C	-2.57713400	1.67311500	0.38100700
C	-2.13862600	1.73174900	-0.98020300
C	-2.57224600	0.54103200	-1.66492000
C	-1.58521300	-0.29015600	-2.31003400
C	-1.69016100	-1.62764800	-1.79576900
C	0.78109500	-1.71873200	-1.53090600
C	0.87664000	-0.54489100	-2.28637100
C	-0.27885500	0.25202600	-2.57423600
C	0.01554100	1.58340800	-2.14615300
C	-0.83643000	2.27547900	-1.27018300
C	0.02071300	2.66994700	-0.16693500
C	-0.30632300	2.34164900	1.16894800
C	0.86176100	1.70267200	1.71386400
C	0.75892300	0.41477900	2.24183000
C	1.73241200	-0.37651200	1.51713700
C	1.30795900	-1.62432500	0.89975200
C	1.72274400	-1.51905500	-0.43095300
C	2.51349100	-0.28696700	-0.59659000
C	1.94682700	0.33056700	-1.69083200
C	1.42340500	1.65832500	-1.62918300
C	1.41003300	2.32571900	-0.43701900
C	2.11201100	1.86707100	0.82637600
C	2.62315500	0.39838500	0.71222000
C	-2.21448700	-2.23643200	0.40075100
C	-2.22267400	-1.54978900	1.63167600
C	-2.75730100	-0.23370300	1.71109800
C	-3.28601800	0.39151900	0.55953500
C	-3.27720300	-0.29799100	-0.69233100
C	-2.73806300	-1.61327900	-0.76920100
H	5.92081600	0.18521700	0.77740500
H	5.37317000	-1.21740900	1.49118500
N	5.21146100	-0.55003400	0.73371000
B	5.03901600	-1.17487700	-0.63822500
H	4.70647000	-2.30873900	-0.67035800
H	5.33664300	-0.50988700	-1.56809600
H	4.19011000	-0.04301400	0.94894400
Li	-1.18829400	-0.23560400	0.07679600
H	2.83934400	2.58442400	1.22101400

$Li@C_{36}^{6-5}1$

1 1

C	0.19826000	-2.31193700	1.07541000
C	0.58775600	-2.66379000	-0.24765300
C	-0.10015800	-2.05965900	-1.34905200
C	0.85990800	-1.39782000	-2.18195000
C	0.72965500	-0.01393800	-2.52089800
C	1.93902500	0.66417200	-2.15151500
C	1.85173200	1.77190800	-1.26274000
C	2.70521500	1.50700000	-0.11159100
C	2.15598200	1.53712200	1.21624800
C	2.43761600	0.28389200	1.86997600

C	1.33084100	-0.49383700	2.37779200
C	1.36533900	-1.80065300	1.78045200
C	-1.07747100	-1.68147400	1.27296000
C	-1.13959700	-0.54626500	2.11131500
C	0.05722300	0.13886900	2.55829100
C	-0.10115300	1.50796600	2.20654100
C	0.87344900	2.15318400	1.40796700
C	0.17012700	2.69356400	0.25619200
C	0.57305100	2.39860100	-1.07181300
C	-0.59251800	1.93241000	-1.80164400
C	-0.53279800	0.65510700	-2.33265200
C	-1.64248000	-0.12661800	-1.73832400
C	-1.38572200	-1.44943700	-1.12477100
C	-1.95389300	-1.42576800	0.13840200
C	-2.78105100	-0.14317100	0.33735800
C	-2.01185600	0.41935300	1.47877200
C	-1.43535400	1.69094200	1.57704900
C	-1.22462600	2.37622000	0.38228800
C	-1.87582500	2.08952200	-0.94922900
C	-2.37324000	0.64578200	-0.89596500
C	2.02442600	-2.33052600	-0.38378000
C	2.19847800	-1.59186500	-1.57440600
C	2.83579700	-0.32846400	-1.52740200
C	3.32008100	0.19624400	-0.29653800
C	3.15163900	-0.55557400	0.90791000
C	2.49841300	-1.82417800	0.85993500
H	-4.92455900	-0.68849800	-1.45806300
H	-6.06593900	-1.23123000	-0.40299100
N	-5.05819400	-1.14244100	-0.55121300
B	-4.40985700	-0.30153100	0.68041700
Li	1.13453300	-0.21884900	0.03381700
H	-2.59199500	2.84848400	-1.28396900
H	-4.67860100	-2.08977700	-0.61897300
H	-4.93472500	0.77940800	0.68842700
H	-4.56875900	-0.95839900	1.67290700

$Li@C_{36}^{6-5}$

11			
C	0.92645800	-2.31238700	-0.78659700
C	1.72470900	-1.46092000	-1.62482500
C	1.08503700	-0.39592200	-2.35034200
C	1.72269200	0.84803700	-2.01391500
C	0.92354100	1.92785800	-1.50254700
C	1.44639600	2.32749000	-0.23030000
C	0.58833500	2.32527900	0.91893300
C	1.17809700	1.50811200	1.93221200
C	0.42660300	0.41772400	2.46970900
C	1.17941500	-0.78874100	2.31888000
C	0.59088000	-1.89314900	1.63036900
C	1.45040600	-2.27335200	0.54622100
C	-0.50129300	-2.35610500	-0.98025200
C	-1.36504800	-2.24968400	0.17280900
C	-0.84121100	-1.91491400	1.44561900

C	-1.63713800	-0.82223800	1.89875300
C	-1.01086900	0.38555100	2.28520900
C	-1.63777200	1.39859300	1.52323000
C	-0.84329700	2.28326500	0.73641200
C	-1.36715600	2.18014000	-0.57514200
C	-0.50370900	1.90380500	-1.69975900
C	-1.09116000	0.77266300	-2.29185900
C	-0.34659700	-0.42474500	-2.51329800
C	-1.09044300	-1.48395900	-1.91090300
C	-2.39058700	-0.96109400	-1.35639900
C	-2.57021000	-1.46023100	-0.10728000
C	-2.93345500	-0.61928000	1.09802800
C	-2.93414500	0.94403600	0.83363100
C	-2.57162800	1.34220900	-0.58101500
C	-2.39112900	0.45970600	-1.59662300
C	2.76593600	-0.85056600	-0.78099700
C	2.76486300	0.54882300	-1.01695700
C	2.60386100	1.45549700	0.07271400
C	2.43705400	0.95788900	1.38393400
C	2.43760300	-0.44745400	1.62161600
C	2.60479200	-1.34817700	0.54651100
Li	0.89645400	-0.00834800	0.01434200
H	-3.83390100	-0.93653100	1.63029900
H	-3.83443600	1.41903400	1.23197800