SUPPORTING INFORMATION

Quantum Mechanical Design and Structures of Hexanuclear Sandwich Complex and its Multidecker Sandwich Clusters $(Li_6)_n$([18]Annulene)$_{n+1}$ (n = 1-3)

Shu-Jian Wang[a*], Ying Li[a], Di Wu[a*], Yin-Feng Wang[b], Zhi-Ru Li[a]

[a] Institute of Theoretical Chemistry, State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, Changchun 130023, People's Republic of China

[b] Jiangxi Province Key Laboratory of Coordination Chemistry, Institute of Applied Chemistry, School of Chemistry and Chemical Engineering, Jinggangshan University, Ji'an, Jiangxi 343009, China

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TABLE S1. Optimized geometries of C_2 and D_{6h} [18]Annulene at CAM-B3LYP/6-31+G(d) and comparison of C-C bond lengths [Å] for those computed at different levels of theory with the X-ray [a] [18]Annulene structure.

[18]Annulene	PG	E_{rel}	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
CAM-B3LYP/6-31+G(d)	D_{6h}	2.9	1.392	1.406	1.392	1.392	1.406	1.392	1.392	1.406	1.392
			C10-C11	C11-C12	C12-C13	C13-C14	C14-C15	C15-C16	C16-C17	C17-C18	C18-C1
			1.392	1.406	1.392	1.392	1.406	1.392	1.392	1.406	1.392
[18]Annulene	PG	E_{rel}	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
CAM-B3LYP/6-31+G(d)	C_2	0	1.438	1.364	1.438	1.355	1.454	1.355	1.438	1.364	1.438
			C10-C11	C11-C12	C12-C13	C13-C14	C14-C15	C15-C16	C16-C17	C17-C18	C18-C1
			1.355	1.454	1.355	1.438	1.364	1.438	1.355	1.454	1.355

		internal bond length	external bond length
experiment (X-ray) [a]	D_{6h}	1.385	1.405
CAM-B3LYP/6-31+G(d)	D_{6h}	1.392	1.406
B3LYP/6-311+G(d, p) [b]	D_{6h}	1.393	1.410
50:50 inversion disorder model:			
CAM-B3LYP/6-31+G(d)	C_2	1.396	1.409
KMLYP/6-311+G(d, p) [b]	C_2	1.379	1.392
BHLYP/6-311+G(d, p) [b]	C_2	1.389	1.396

PG is the point group. E_{rel} [kcal/mol] is the relative energy with respect to the energetically most stable structure, at various levels of theory. Positive values of E_{rel} indicate that the C_2 structure is more stable than D_{6h} structure. [a] Ref 19. [b] Ref 17c. It has been reported in Ref 17c that the X-ray structure determination fail to find the correct geometry, and a possible reason is static disorder. A superposition of a lower symmetry structure can lead to apparent higher symmetry, i.e. 50:50 inversion disorder model of bond alternating C_2 structures can lead to a apparent higher D_{6h} symmetrical structures.

TABLE S2. Comparison of C···C major and minor interatomic distances [Å] across the [18]Annulene ring for those computed at different levels of theory with the X-ray [a] [18]Annulene structure.

		C···C across the ring	
		Minor	Major
experiment (X-ray) [a]	D_{6h}	5.91	7.54
CAM-B3LYP/6-31+G*	D_{6h}	5.94	7.58
B3LYP/6-311+G(d, p) [b]	D_{6h}	5.96	7.6
KMLYP/6-311+G(d, p) [b]	D_{6h}	5.86	7.48
50:50 inversion disorder model of bond alternating C_2 structures			
CAM-B3LYP/6-31+G(d)	C_2	5.95	7.58
KMLYP/6-311+G(d, p) [b]	C_2	5.86	7.48
BHLYP/6-311+G(d, p) [b]	C_2	5.92	7.54

[a] Ref 19. [b] Ref 17c. It has been reported in Ref 17c that the X-ray structure determination fail to find the correct geometry, and a possible reason is static disorder. A superposition of a lower symmetry structure can lead to apparent higher symmetry, i.e. 50:50 inversion disorder model of bond alternating C_2 structures can lead to a apparent higher D_{6h} symmetrical structures.

TABLE S3. Calculated bond dissociation energies BDE for dissociation of $FeCp_2$ (ferrocene) into Fe and two Cp ligands.

Reaction	D_e	D_o	Exp.
$FeCp_2 \rightarrow Fe(3d^6 4s^2)\ ^5D + 2Cp$	137.3	131.5	158±2 [a]

D_e is the bond dissociation energies BDE without ZPE corrections, D_o is the bond dissociation energies BDE with ZPE corrections. $FeCp_2$ (ferrocene) has an equilibrium geometry with D_{5h} symmetry, neutral fragments Fe has a $(3d^6 4s^2)\ ^5D$ ground state. The bond dissociation energies were obtained at the CAM-B3LYP/gen level with the lanl2dz basis set including a corrected effective core potential (ECP) to take into account relativistic effects for Fe and 6-31G* basis set for C and H. [a] Ref 22.

TABLE S4. Bond dissociation energies BDE for dissociation of lithium-benzene sandwich complex $Li\cdot(C_6H_6)_2$ into Li and two C_6H_6 using various methods.

$Li\cdot(C_6H_6)_2 \rightarrow Li + 2C_6H_6$	D_e	D_o
CAM-B3LYP/6-31G(d)//CAM-B3LYP/6-31G(d)	15.8	18.0
MP2/6-31G(d)//MP2/6-31G(d) [a]	19.6	
QCISD(T)/6-31G(d)//MP2/6-31G(d) [a]	15.5	
G3(MP2) [a]	22.4	19.6

D_e is the bond dissociation energies BDE without ZPE corrections, D_o is the bond dissociation energies BDE with ZPE corrections. $Li\cdot(C_6H_6)_2$ has an equilibrium geometry with C_{2v} symmetry at CAM-B3LYP level of theory. [a] The BDE data of the D_{2h} structure of $Li\cdot(C_6H_6)_2$ at various methods is from Ref 32.

TABLE S5. Details of the geometrical structure for the hexanuclear sandwich complex [18]Annulene-Li_6-[18]Annulene with C_2 symmetry.

[18]Annulene-Li_6-[18]Annulene	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10
C-C bond length	1.422	1.393	1.425	1.393	1.419	1.399	1.412	1.414	1.407
	C10-C11	C11-C12	C12-C13	C13-C14	C14-C15	C15-C16	C16-C17	C17-C18	C18-C1
	1.407	1.435	1.388	1.431	1.438	1.382	1.442	1.409	1.402
layer distance L [a]	C1-C1'	C2-C2'	C3-C3'	C4-C4'	C5-C5'	C6-C6'	C7-C7'	C8-C8'	C9-C9'
	3.744	3.753	3.742	3.746	3.737	3.730	3.721	3.731	3.689
R_{Li-Li} [b]	LI1-LI2	LI2-LI3	LI3-LI4	LI4-LI5	LI5-LI6	LI6-LI1			
	2.900	2.851	2.872	2.872	2.851	2.900			

[a] the averaged layer distance L is 3.732 Å. [b] the averaged distance between two lithium atoms is 2.874 Å.

TABLE S6. NBO charges of lithium atoms and WBI of Li-Li bond in the hexanuclear sandwich complex, and CDA results from back-donation between two [18]Annulene^{2-} ligand fragments and metal Li_6^{4+} ring fragment.

NBO [a]	Li1	Li2	Li3	Li4	Li5	Li6
	0.476	0.469	0.454	0.449	0.454	0.469
WBI [a]	Li1-Li2	Li2-Li3	Li3-Li4	Li4-Li5	Li5-Li6	Li6-Li1
	0.0448	0.0490	0.0497	0.0497	0.0490	0.0448
CDA [b]	Ligand 1→Li_6	Li_6→Ligand 1	Ligand 1↔Li_6	Ligand 2→Li_6	Li_6→Ligand 2	Ligand 2↔Li_6
	d	b	r	d	b	r
	3.498	0.105	-0.134	3.498	0.105	-0.134

[a] NBO charges and WBI are obtained at the CAM-B3LYP/6-31+G* level, the sum of NBO charges of lithium atoms is +2.770 e. [b] CDA results are obtained at the CAM-B3LYP/6-31G* level on the CAM-B3LYP/6-31+G* geometry. Definitions: donation (d), back-donation (b), and repulsive polarization (r).

Cartesian coordinate for $(Li_6)_n$([18]Annulene)$_{n+1}$ (n = 1-3)

[18]Annulene-Li_6-[18]Annulene with C_2 symmetry at the CAM-B3LYP/6-31+G* level

C	-0.61184400	1.89869600	3.78077800
C	0.00000000	2.41989400	2.60724100
C	-2.30436100	0.54213000	2.54900000
C	-1.71464300	1.03408800	3.72979000
C	-2.33337100	0.53935900	-2.57551700
C	-3.46479400	-0.33932800	-2.48671100
C	-3.98893500	-0.74915300	-1.26901700
C	-3.43995700	-0.36943400	-0.00357000
C	-3.99251200	-0.73832300	1.27182400
C	-3.45798000	-0.32049900	2.47534400
H	-3.89756400	-0.68186800	3.40239000
H	-4.83441500	-1.42844600	1.29122800
H	-0.20491300	2.16769500	4.75208900
H	-2.09469000	0.66106800	4.68033800
H	-3.90165700	-0.72533900	-3.40482200
H	-4.81803400	-1.45516700	-1.28024600
C	1.11900200	3.24084400	2.49275100
C	1.67406200	3.68008100	1.25639300
C	1.17101000	3.33816700	0.00322700
H	1.63335700	3.54742900	3.40146900
H	2.57418200	4.28967200	1.30607800
C	1.67890100	3.67750600	-1.27802600
C	1.11780000	3.22735700	-2.47840400
C	-0.00081500	2.37092200	-2.57893600
H	2.56679000	4.30312500	-1.33350800
H	1.61219200	3.52603000	-3.40134100
C	-1.70888000	1.00549700	-3.74669200
H	-2.06339800	0.63298800	-4.70618700
C	-0.60015000	1.87113400	-3.75818000
H	-0.16162200	2.13140500	-4.71883700
H	-2.85446400	0.54312100	-0.00591100
H	-2.08247500	1.06589200	-1.66160700
H	-0.55224300	2.20215800	-1.65961800
H	0.22677800	2.80039300	0.00154600
H	-0.53134900	2.21612700	1.68170200
H	-2.06009700	1.07193400	1.63526900
C	1.71464300	-1.03408800	3.72979000
C	2.30436100	-0.54213000	2.54900000

C	0.00000000	-2.41989400	2.60724100
C	0.61184400	-1.89869600	3.78077800
C	0.00081500	-2.37092200	-2.57893600
C	-1.11780000	-3.22735700	-2.47840400
C	-1.67890100	-3.67750600	-1.27802600
C	-1.17101000	-3.33816700	0.00322700
C	-1.67406200	-3.68008100	1.25639300
C	-1.11900200	-3.24084400	2.49275100
H	-1.63335700	-3.54742900	3.40146900
H	-2.57418200	-4.28967200	1.30607800
H	2.09469000	-0.66106800	4.68033800
H	0.20491300	-2.16769500	4.75208900
H	-1.61219200	-3.52603000	-3.40134100
H	-2.56679000	-4.30312500	-1.33350800
C	3.45798000	0.32049900	2.47534400
C	3.99251200	0.73832300	1.27182400
C	3.43995700	0.36943400	-0.00357000
H	3.89756400	0.68186800	3.40239000
H	4.83441500	1.42844600	1.29122800
C	3.98893500	0.74915300	-1.26901700
C	3.46479400	0.33932800	-2.48671100
C	2.33337100	-0.53935900	-2.57551700
H	4.81803400	1.45516700	-1.28024600
H	3.90165700	0.72533900	-3.40482200
C	0.60015000	-1.87113400	-3.75818000
H	0.16162200	-2.13140500	-4.71883700
C	1.70888000	-1.00549700	-3.74669200
H	2.06339800	-0.63298800	-4.70618700
H	-0.22677800	-2.80039300	0.00154600
H	0.55224300	-2.20215800	-1.65961800
H	2.08247500	-1.06589200	-1.66160700
H	2.85446400	-0.54312100	-0.00591100
H	2.06009700	-1.07193400	1.63526900
H	0.53134900	-2.21612700	1.68170200
Li	0.00000000	0.00000000	2.90049400
Li	-2.01129900	-1.47831400	1.42522000
Li	-2.00770800	-1.48007600	-1.42621800
Li	0.00000000	0.00000000	-2.85036900
Li	2.00770800	1.48007600	-1.42621800
Li	2.01129900	1.47831400	1.42522000

[18]Annulene-Li_6-[18]Annulene with C_{2h} symmetry at the B3LYP/6-31G* level

C	0.70010000	1.84448900	3.77184100
C	1.48915700	1.89855400	2.59180100
C	-1.49790400	1.89373200	2.59248700
C	-0.70708600	1.84025100	3.77137000
C	-1.49790400	1.89373200	-2.59248700
C	-2.91538800	1.83851400	-2.49771100
C	-3.61670500	1.85377200	-1.27742300
C	-2.98850300	1.89124100	0.00000000
C	-3.61670500	1.85377200	1.27742300
C	-2.91538800	1.83851400	2.49771100
H	-3.49365100	1.73325600	3.41420000
H	-4.70140400	1.76522600	1.31603900
H	1.20695100	1.74269100	4.73017000
H	-1.21310500	1.73219300	4.72955200
H	-3.49365100	1.73325600	-3.41420000
H	-4.70140400	1.76522600	-1.31603900
C	2.90437400	1.84874900	2.49253300
C	3.60575400	1.86066100	1.27311100
C	2.97717200	1.91621800	0.00000000
H	3.48310600	1.74385400	3.40901600
H	4.68955700	1.76125200	1.31042500
C	3.60575400	1.86066100	-1.27311100
C	2.90437400	1.84874900	-2.49253300
C	1.48915700	1.89855400	-2.59180100
H	4.68955700	1.76125200	-1.31042500
H	3.48310600	1.74385400	-3.40901600
C	-0.70708600	1.84025100	-3.77137000
H	-1.21310500	1.73219300	-4.72955200
C	0.70010000	1.84448900	-3.77184100
H	1.20695100	1.74269100	-4.73017000
H	-1.93082100	2.13244800	0.00000000
H	-0.97466400	2.17904400	-1.68538700
H	0.95942800	2.16274700	-1.68239600
H	1.92569500	2.19082300	0.00000000
H	0.95942800	2.16274700	1.68239600
H	-0.97466400	2.17904400	1.68538700
C	0.70708600	-1.84025100	3.77137000
C	1.49790400	-1.89373200	2.59248700
C	-1.48915700	-1.89855400	2.59180100
C	-0.70010000	-1.84448900	3.77184100

C	-1.48915700	-1.89855400	-2.59180100
C	-2.90437400	-1.84874900	-2.49253300
C	-3.60575400	-1.86066100	-1.27311100
C	-2.97717200	-1.91621800	0.00000000
C	-3.60575400	-1.86066100	1.27311100
C	-2.90437400	-1.84874900	2.49253300
H	-3.48310600	-1.74385400	3.40901600
H	-4.68955700	-1.76125200	1.31042500
H	1.21310500	-1.73219300	4.72955200
H	-1.20695100	-1.74269100	4.73017000
H	-3.48310600	-1.74385400	-3.40901600
H	-4.68955700	-1.76125200	-1.31042500
C	2.91538800	-1.83851400	2.49771100
C	3.61670500	-1.85377200	1.27742300
C	2.98850300	-1.89124100	0.00000000
H	3.49365100	-1.73325600	3.41420000
H	4.70140400	-1.76522600	1.31603900
C	3.61670500	-1.85377200	-1.27742300
C	2.91538800	-1.83851400	-2.49771100
C	1.49790400	-1.89373200	-2.59248700
H	4.70140400	-1.76522600	-1.31603900
H	3.49365100	-1.73325600	-3.41420000
C	-0.70010000	-1.84448900	-3.77184100
H	-1.20695100	-1.74269100	-4.73017000
C	0.70708600	-1.84025100	-3.77137000
H	1.21310500	-1.73219300	-4.72955200
H	-1.92569500	-2.19082300	0.00000000
H	-0.95942800	-2.16274700	-1.68239600
H	0.97466400	-2.17904400	-1.68538700
H	1.93082100	-2.13244800	0.00000000
H	0.97466400	-2.17904400	1.68538700
H	-0.95942800	-2.16274700	1.68239600
Li	0.00000000	0.00000000	2.81822100
Li	-2.46744400	0.01489500	1.36715500
Li	-2.46744400	0.01489500	-1.36715500
Li	0.00000000	0.00000000	-2.81822100
Li	2.46744400	-0.01489500	-1.36715500
Li	2.46744400	-0.01489500	1.36715500

$(Li_6)_2$([18]Annulene)$_3$ with C_{2v} symmetry at the B3LYP/6-31G* level

C	-3.61343000	3.98123700	1.27674300

C	-2.98946400	3.88784700	0.00000000
C	-1.51214900	3.92391800	2.63307700
C	-2.93749400	3.97161500	2.50993500
C	2.98698500	3.89006000	0.00000000
C	3.61087500	3.98427700	1.27673500
C	2.93497400	3.97412600	2.50993000
C	1.50965500	3.92508900	2.63308200
C	0.71489200	3.95464100	3.79027700
C	-0.71741300	3.95400500	3.79028000
H	-1.21302100	3.96332500	4.76080000
H	1.21049000	3.96446100	4.76079900
H	-4.70222600	4.03394500	1.30507100
H	-3.53423300	4.01572000	3.41977000
H	4.69961600	4.03816900	1.30503500
H	3.53166800	4.01901300	3.41975700
C	-3.61343000	3.98123700	-1.27674300
C	-2.93749400	3.97161500	-2.50993500
C	-1.51214900	3.92391800	-2.63307700
H	-4.70222600	4.03394500	-1.30507100
H	-3.53423300	4.01572000	-3.41977000
C	-0.71741300	3.95400500	-3.79028000
C	0.71489200	3.95464100	-3.79027700
C	1.50965500	3.92508900	-2.63308200
H	-1.21302100	3.96332500	-4.76080000
H	1.21049000	3.96446100	-4.76079900
C	3.61087500	3.98427700	-1.27673500
H	4.69961600	4.03816900	-1.30503500
C	2.93497400	3.97412600	-2.50993000
H	3.53166800	4.01901300	-3.41975700
H	0.96886700	4.03643600	1.69470100
H	1.90321300	3.98532900	0.00000000
H	0.96886700	4.03643600	-1.69470100
H	-0.97145800	4.03589500	-1.69471800
H	-1.90579600	3.98429600	0.00000000
H	-0.97145800	4.03589500	1.69471800
C	-3.64054500	0.00000100	1.28741700
C	-3.00029500	0.00033000	0.00000000
C	-1.49733900	-0.00237100	2.59463800
C	-2.93930100	-0.00112000	2.50515900
C	3.00100800	0.00259100	0.00000000
C	3.64124700	0.00229900	1.28739200

C	2.94002600	0.00089300	2.50514700
C	1.49806000	-0.00118900	2.59461500
C	0.70781500	-0.00279200	3.78888600
C	-0.70706600	-0.00317900	3.78892700
H	-1.21860400	-0.00524800	4.74951500
H	1.21938400	-0.00456100	4.74945500
H	-4.72878500	0.00108800	1.32342100
H	-3.51301400	-0.00173700	3.42984600
H	4.72948400	0.00347500	1.32338200
H	3.51373700	0.00034800	3.42983400
C	-3.64054500	0.00000100	-1.28741700
C	-2.93930100	-0.00112000	-2.50515900
C	-1.49733900	-0.00237100	-2.59463800
H	-4.72878500	0.00108800	-1.32342100
H	-3.51301400	-0.00173700	-3.42984600
C	-0.70706600	-0.00317900	-3.78892700
C	0.70781500	-0.00279200	-3.78888600
C	1.49806000	-0.00118900	-2.59461500
H	-1.21860400	-0.00524800	-4.74951500
H	1.21938400	-0.00456100	-4.74945500
C	3.64124700	0.00229900	-1.28739200
H	4.72948400	0.00347500	-1.32338200
C	2.94002600	0.00089300	-2.50514700
H	3.51373700	0.00034800	-3.42983400
H	0.95604200	0.00209600	1.64961600
H	1.91200200	0.00017800	0.00000000
H	0.95604200	0.00209600	-1.64961600
H	-0.95532800	0.00149000	-1.64964100
H	-1.91129700	-0.00301600	0.00000000
H	-0.95532800	0.00149000	1.64964100
Li	-2.73322500	2.01350600	1.56342200
Li	-0.00009000	1.99743900	3.12887300
Li	2.73299700	2.01558500	1.56368900
Li	2.73299700	2.01558500	-1.56368900
Li	-0.00009000	1.99743900	-3.12887300
Li	-2.73322500	2.01350600	-1.56342200
C	-3.61059300	-3.98344000	1.27663600
C	-2.98654800	-3.88768500	0.00000000
C	-1.50982800	-3.92653300	2.63347800
C	-2.93529200	-3.97364600	2.50999700
C	2.98845200	-3.88528300	0.00000000

C	3.61256200	-3.98005200	1.27661500
C	2.93721300	-3.97092100	2.51000400
C	1.51175600	-3.92529000	2.63349000
C	0.71727500	-3.95309900	3.79057000
C	-0.71532500	-3.95384700	3.79055300
H	-1.21081300	-3.96062700	4.76114500
H	1.21275400	-3.95931700	4.76116500
H	-4.69932100	-4.03793000	1.30447700
H	-3.53234300	-4.01831800	3.41958800
H	4.70135100	-4.03325800	1.30449100
H	3.53433000	-4.01476400	3.41959300
C	-3.61059300	-3.98344000	-1.27663600
C	-2.93529200	-3.97364600	-2.50999700
C	-1.50982800	-3.92653300	-2.63347800
H	-4.69932100	-4.03793000	-1.30447700
H	-3.53234300	-4.01831800	-3.41958800
C	-0.71532500	-3.95384700	-3.79055300
C	0.71727500	-3.95309900	-3.79057000
C	1.51175600	-3.92529000	-2.63349000
H	-1.21081300	-3.96062700	-4.76114500
H	1.21275400	-3.95931700	-4.76116500
C	3.61256200	-3.98005200	-1.27661500
H	4.70135100	-4.03325800	-1.30449100
C	2.93721300	-3.97092100	-2.51000400
H	3.53433000	-4.01476400	-3.41959300
H	0.97120400	-4.03902600	1.69524600
H	1.90455500	-3.97932000	0.00000000
H	0.97120400	-4.03902600	-1.69524600
H	-0.96917400	-4.03965300	-1.69521600
H	-1.90256200	-3.98070600	0.00000000
H	-0.96917400	-4.03965300	1.69521600
Li	-2.73419800	-2.01407400	1.56239600
Li	-0.00084900	-1.99951000	3.12099100
Li	2.73386100	-2.01151500	1.56297600
Li	2.73386100	-2.01151500	-1.56297600
Li	-0.00084900	-1.99951000	-3.12099100
Li	-2.73419800	-2.01407400	-1.56239600

$(Li_6)_3$([18]Annulene)$_4$ with C_{2h} symmetry at the B3LYP/6-31G* level

C	-3.63952900	1.97629100	1.28869100
C	-2.99707800	1.94789700	0.00000000

C	-1.49795600	1.97138200	2.59675100
C	-2.93797700	1.98266600	2.50686700
C	2.99843600	1.95503800	0.00000000
C	3.64082200	1.98321800	1.28873300
C	2.93894900	1.98859600	2.50678700
C	1.49885700	1.97514400	2.59644600
C	0.70580800	1.99120900	3.79463700
C	-0.70496500	1.99021100	3.79468000
H	-1.21759900	2.01844100	4.75462700
H	1.21855000	2.02017500	4.75451100
H	-4.72773400	1.99097300	1.32359100
H	-3.51268200	2.01010100	3.43088600
H	4.72903400	1.99756200	1.32390700
H	3.51343400	2.01547200	3.43097400
C	-3.63952900	1.97629100	-1.28869100
C	-2.93797700	1.98266600	-2.50686700
C	-1.49795600	1.97138200	-2.59675100
H	-4.72773400	1.99097300	-1.32359100
H	-3.51268200	2.01010100	-3.43088600
C	-0.70496500	1.99021100	-3.79468000
C	0.70580800	1.99120900	-3.79463700
C	1.49885700	1.97514400	-2.59644600
H	-1.21759900	2.01844100	-4.75462700
H	1.21855000	2.02017500	-4.75451100
C	3.64082200	1.98321800	-1.28873300
H	4.72903400	1.99756200	-1.32390700
C	2.93894900	1.98859600	-2.50678700
H	3.51343400	2.01547200	-3.43097400
H	0.95581400	1.96644100	1.65265700
H	1.91058300	2.00908600	0.00000000
H	0.95581400	1.96644100	-1.65265700
H	-0.95484100	1.96358700	-1.65299800
H	-1.90903800	1.99768800	0.00000000
H	-0.95484100	1.96358700	1.65299800
C	-3.64082200	-1.98321800	1.28873300
C	-2.99843600	-1.95503800	0.00000000
C	-1.49885700	-1.97514400	2.59644600
C	-2.93894900	-1.98859600	2.50678700
C	2.99707800	-1.94789700	0.00000000
C	3.63952900	-1.97629100	1.28869100
C	2.93797700	-1.98266600	2.50686700

C	1.49795600	-1.97138200	2.59675100
C	0.70496500	-1.99021100	3.79468000
C	-0.70580800	-1.99120900	3.79463700
H	-1.21855000	-2.02017500	4.75451100
H	1.21759900	-2.01844100	4.75462700
H	-4.72903400	-1.99756200	1.32390700
H	-3.51343400	-2.01547200	3.43097400
H	4.72773400	-1.99097300	1.32359100
H	3.51268200	-2.01010100	3.43088600
C	-3.64082200	-1.98321800	-1.28873300
C	-2.93894900	-1.98859600	-2.50678700
C	-1.49885700	-1.97514400	-2.59644600
H	-4.72903400	-1.99756200	-1.32390700
H	-3.51343400	-2.01547200	-3.43097400
C	-0.70580800	-1.99120900	-3.79463700
C	0.70496500	-1.99021100	-3.79468000
C	1.49795600	-1.97138200	-2.59675100
H	-1.21855000	-2.02017500	-4.75451100
H	1.21759900	-2.01844100	-4.75462700
C	3.63952900	-1.97629100	-1.28869100
H	4.72773400	-1.99097300	-1.32359100
C	2.93797700	-1.98266600	-2.50686700
H	3.51268200	-2.01010100	-3.43088600
H	0.95484100	-1.96358700	1.65299800
H	1.90903800	-1.99768800	0.00000000
H	0.95484100	-1.96358700	-1.65299800
H	-0.95581400	-1.96644100	-1.65265700
H	-1.91058300	-2.00908600	0.00000000
H	-0.95581400	-1.96644100	1.65265700
Li	-2.71727700	-0.00388200	1.55260500
Li	0.00000000	0.00000000	3.15301000
Li	2.71727700	0.00388200	1.55260500
Li	2.71727700	0.00388200	-1.55260500
Li	0.00000000	0.00000000	-3.15301000
Li	-2.71727700	-0.00388200	-1.55260500
C	-3.61786600	5.94068300	1.27764400
C	-2.99081500	5.84738900	0.00000000
C	-1.51446900	5.90201400	2.62923000
C	-2.94119200	5.93708700	2.50918100
C	2.98349400	5.85515600	0.00000000
C	3.61007100	5.95356300	1.27757400

C	2.93346000	5.94815600	2.50905400
C	1.50675500	5.90668500	2.62916100
C	0.71162800	5.92479000	3.78801400
C	-0.71940400	5.92167200	3.78802100
H	-1.21548200	5.91418500	4.75853400
H	1.20779700	5.91986700	4.75851100
H	-4.70735200	5.97980000	1.30558000
H	-3.53699600	5.97039400	3.42030400
H	4.69931800	5.99904600	1.30541200
H	3.52902600	5.98620400	3.42015000
C	-3.61786600	5.94068300	-1.27764400
C	-2.94119200	5.93708700	-2.50918100
C	-1.51446900	5.90201400	-2.62923000
H	-4.70735200	5.97980000	-1.30558000
H	-3.53699600	5.97039400	-3.42030400
C	-0.71940400	5.92167200	-3.78802100
C	0.71162800	5.92479000	-3.78801400
C	1.50675500	5.90668500	-2.62916100
H	-1.21548200	5.91418500	-4.75853400
H	1.20779700	5.91986700	-4.75851100
C	3.61007100	5.95356300	-1.27757400
H	4.69931800	5.99904600	-1.30541200
C	2.93346000	5.94815600	-2.50905400
H	3.52902600	5.98620400	-3.42015000
H	0.96763100	6.03542400	1.69245200
H	1.90200400	5.96934100	0.00000000
H	0.96763100	6.03542400	-1.69245200
H	-0.97592200	6.03411800	-1.69268000
H	-1.91006400	5.96828600	0.00000000
H	-0.97592200	6.03411800	1.69268000
Li	-2.69962900	3.99314500	1.54063300
Li	0.00486400	3.98421200	3.08371700
Li	2.70363600	4.00119300	1.54284500
Li	2.70363600	4.00119300	-1.54284500
Li	0.00486400	3.98421200	-3.08371700
Li	-2.69962900	3.99314500	-1.54063300
C	-3.61007100	-5.95356300	1.27757400
C	-2.98349400	-5.85515600	0.00000000
C	-1.50675500	-5.90668500	2.62916100
C	-2.93346000	-5.94815600	2.50905400
C	2.99081500	-5.84738900	0.00000000

C	3.61786600	-5.94068300	1.27764400
C	2.94119200	-5.93708700	2.50918100
C	1.51446900	-5.90201400	2.62923000
C	0.71940400	-5.92167200	3.78802100
C	-0.71162800	-5.92479000	3.78801400
H	-1.20779700	-5.91986700	4.75851100
H	1.21548200	-5.91418500	4.75853400
H	-4.69931800	-5.99904600	1.30541200
H	-3.52902600	-5.98620400	3.42015000
H	4.70735200	-5.97980000	1.30558000
H	3.53699600	-5.97039400	3.42030400
C	-3.61007100	-5.95356300	-1.27757400
C	-2.93346000	-5.94815600	-2.50905400
C	-1.50675500	-5.90668500	-2.62916100
H	-4.69931800	-5.99904600	-1.30541200
H	-3.52902600	-5.98620400	-3.42015000
C	-0.71162800	-5.92479000	-3.78801400
C	0.71940400	-5.92167200	-3.78802100
C	1.51446900	-5.90201400	-2.62923000
H	-1.20779700	-5.91986700	-4.75851100
H	1.21548200	-5.91418500	-4.75853400
C	3.61786600	-5.94068300	-1.27764400
H	4.70735200	-5.97980000	-1.30558000
C	2.94119200	-5.93708700	-2.50918100
H	3.53699600	-5.97039400	-3.42030400
H	0.97592200	-6.03411800	1.69268000
H	1.91006400	-5.96828600	0.00000000
H	0.97592200	-6.03411800	-1.69268000
H	-0.96763100	-6.03542400	-1.69245200
H	-1.90200400	-5.96934100	0.00000000
H	-0.96763100	-6.03542400	1.69245200
Li	-2.70363600	-4.00119300	1.54284500
Li	-0.00486400	-3.98421200	3.08371700
Li	2.69962900	-3.99314500	1.54063300
Li	2.69962900	-3.99314500	-1.54063300
Li	-0.00486400	-3.98421200	-3.08371700
Li	-2.70363600	-4.00119300	-1.54284500