Supporting Information

Theoretical study on lithiation mechanism of benzoquinone-based macrocyclic compounds as cathode for lithium-ion batteries

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Solvation effect simulation

In the lithiation mechanism investigation of cathode material, the solvation effect is very important and should be considered in the calculations.[S1] So we use the implicit solvent model to describe solvation effect in the lithiation mechanism investigation of the benzoquinone-based macrocyclic compounds. It is no doubt that some side reactions will affect the electrochemical reaction in the batteries system. With regard to the behavior of co-intercalation and the formation of solid electrolyte interphases (SEI), it widely exists in layered inorganic anodes, such as graphite.[S2] However, the co-intercalation has not been found in organic carbonyl cathodes for LIBs and there are still occasional arguments that SEI in traditional sense does not exist on cathode side.[S3] In fact, the reaction mechanism of organic carbonyl compounds as cathode in LIBs is the binding of Li^+ ions with the carbonyl oxygen of cathodes.[S4] As for BQ-based macrocyclic compounds, they are no exception. For the effect of solvation, it is only correlated to the redox potentials and capacity fading which caused by the dissolution of organic cathodes.[S5] Lots of reported literatures use the implicit solvent model to calculate the redox potentials and have achieved credible results.[S6-S8] Therefore, we choose the implicit solvent model (SMD)[S9] in this work. As Donald G. Truhlar *et al*. has pointed out, "A key advantage of the SMD approach is that the non-bulk-electrostatic effects are parametrized to be consistent with a given choice of solute radii. If the solute radii are changed and the parametrization repeated, one obtains similar results; thus the sensitivity to the choice of radii is diminished."[S10] Thus, SMD can also simulate the solvent effect at the interface to some extent.

S1 S. J. Yang, X. Y. Qin, R. He, W. Shen, M. Li and L. B. Zhao, *Phys. Chem. Chem. Phys.*, 2017, **19**, 12480-12489.

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S3 K. Xu and A. von Cresce, *J. Mater. Chem.*, 2011, **21**, 9849.

S4 Y. Wu, R. Zeng, J. Nan, D. Shu, Y. Qiu and S.-L. Chou, *Adv. Energy Mater.*, 2017, **7**, 1700278.

S5 K. C. Kim, T. Liu, S. W. Lee and S. S. Jang, *J. Am. Chem. Soc.*, 2016, **138**, 2374-2382.

S6 D. J. Kim, K. R. Hermann, A. Prokofjevs, M. T. Otley, C. Pezzato, M. Owczarek and J. F. Stoddart, *J. Am. Chem. Soc.*, 2017, **139**, 6635-6643.

S7 D. Wu, Z. Xie, Z. Zhou, P. Shen and Z. Chen, *J. Mater. Chem. A*, 2015, **3**, 19137-19143.

S8 J. H. Park, T. Liu, K. C. Kim, S. W. Lee and S. S. Jang, *ChemSusChem*, 2017, **10**, 1584-1591.

S9 A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.

S10 A. V. Marenich, J. Ho, M. L. Coote, C. J. Cramer and D. G. Truhlar, *Phys. Chem. Chem. Phys.*, 2014, **16**, 15068-15106.

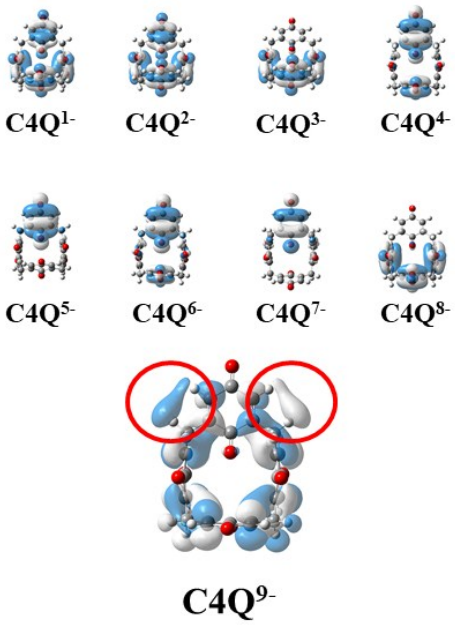

Fig. S1 HOMO diagrams of C4Q with different reduced forms at B3LYP/6-31G(d) (Top view).

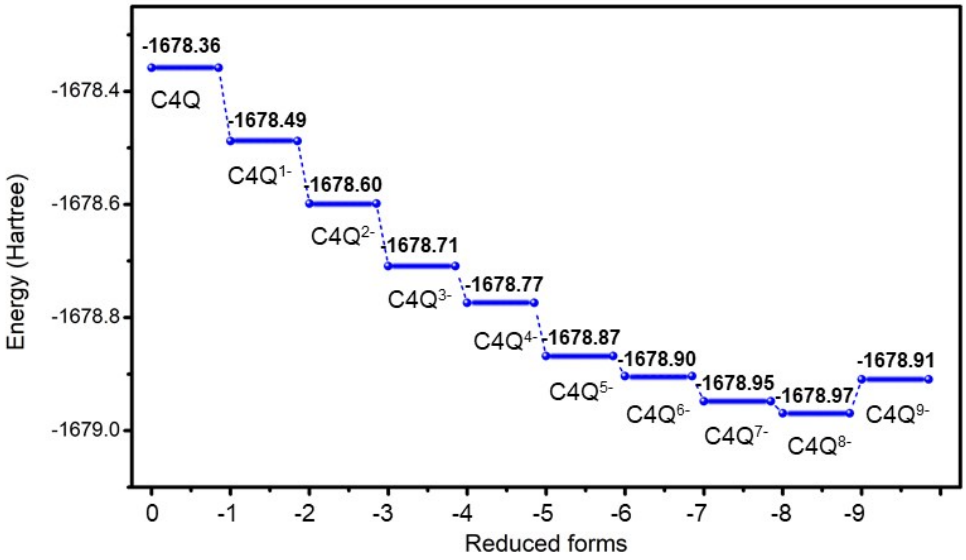

Fig. S2 Energies of C4Q with different reduced forms at B3LYP/6-31G(d)

Table S1. Fukui indices of each oxygen atom in $C4QLi_{0\sim7}$ during the lithiation process.

Species		**Atom**							
		O1	O2	O3	O4	O5	O6	O7	O8
$C4QLi_0$	f_O^+	0.058	0.034	0.034	0.035	0.049	0.049	**0.180**	0.018
$C4QLi_1$	f_O^+	0.022	0.042	0.042	0.012	**0.114**	0.114	0.046	0.001
$C4QLi_2$	f_O^+	0.047	0.034	0.052	0.010	0.038	0.065	**0.087**	-0.077
$C4QLi_3$	f_O^+	0.012	0.023	0.110	0.011	0.030	**0.123**	0.006	-0.048
$C4QLi_4$	f_O^+	0.020	0.083	0.013	0.035	**0.096**	0.007	0.012	-0.045
$C4QLi_5$	f_O^+	0.030	0.018	0.035	**0.064**	0.010	0.040	0.034	0.021
$C4QLi_6$	f_O^+	0.034	0.020	**0.053**	0.047	0.012	0.037	0.040	-0.010
$C4QLi_7$	f_O^+	**0.064**	0.028	0.012	0.025	0.014	0.054	0.055	-0.151

Table S2. Thermal Gibbs free energy change (including zero-point energy) of C4Q in each lithiation step. The ΔG_{IT} (in eV) and ΔG_{ET} (in eV) corresponding to the Gibbs free energy change of ion transfer step and electron transfer step, respectively.

Discharge process	Pattern 1		Pattern 2	
	ΔG_{IT}	ΔG_{ET}	ΔG_{IT}	ΔG_{ET}
$C4Q \rightarrow C4QLi_1$	-0.42	-2.78	-1.23	-1.97
$C4QLi_1 \rightarrow C4QLi_2$	-0.39	-2.56	-1.05	-1.91
$C4QLi_2 \rightarrow C4QLi_3$	-0.32	-2.56	-0.91	-1.97
$C4QLi_3 \rightarrow C4QLi_4$	-0.75	-2.29	-1.71	-1.35
$C4QLi_4 \rightarrow C4QLi_5$	-0.64	-2.29	-0.91	-2.02
$C4QLi_5 \rightarrow C4QLi_6$	-0.72	-2.25	-1.73	-1.25
$C4QLi_6 \rightarrow C4QLi_7$	-0.67	-2.11	-1.38	-1.39
$C4QLi_7 \rightarrow C4QLi_8$	-0.64	-1.85	-1.99	-0.51

Table S3. Fukui indices of each oxygen atom in $P5QLi_{1\sim9}$ during the lithiation process.

Species		Atom									
		O1	O2	O3	O4	O5	O6	O7	O8	O9	O10
$P5QLi_1$	f_O^+	-0.026	**0.114**	0.063	0.040	0	0.065	0.084	0.034	0.002	-0.014
$P5QLi_2$	f_O^+	-0.007	0.087	**0.087**	-0.007	-0.004	0.058	0.058	0.014	-0.004	0.014
$P5QLi_3$	f_O^+	-0.008	**0.086**	0.053	0.018	0.003	0.071	0.068	0.017	0.006	-0.011
$P5QLi_4$	f_O^+	-0.002	0.008	**0.136**	0.037	0.012	0.018	0.085	0.033	0.017	0.001
$P5QLi_5$	f_O^+	0.003	0.007	-0.004	**0.154**	0.027	0.003	0.019	-0.004	0.035	0.004
$P5QLi_6$	f_O^+	0.006	0.005	-0.002	0.027	**0.191**	0.002	0.010	-0.019	0.111	0.006
$P5QLi_7$	f_O^+	0.001	0.003	-0.008	0.101	0.035	0.001	0.006	**0.110**	0.020	0.003
$P5QLi_8$	f_O^+	0.100	0.055	0.001	0.002	0.005	0.061	-0.005	0.005	0.003	**0.133**
$P5QLi_9$	f_O^+	-0.001	**0.187**	0.004	0.001	0.002	0.162	-0.011	0.001	-0.001	0.006

Table S4. Thermal Gibbs free energy change (including zero-point energy) of P5Q in each lithiation step. The ΔG_{IT} (in eV) and ΔG_{ET} (in eV) corresponding to the Gibbs free energy change of ion transfer step and electron transfer step, respectively.

Discharge process	Pattern 1		Pattern 2	
	ΔG_{IT}	ΔG_{ET}	ΔG_{IT}	ΔG_{ET}
$P5QLi \rightarrow P5QLi_1$	-0.04	-2.82	-1.36	-1.5
$P5QLi_1 \rightarrow P5QLi_2$	-1.82	-2.81	-2.65	-1.98
$P5QLi_2 \rightarrow P5QLi_3$	-0.25	-2.70	-1.01	-1.99
$P5QLi_3 \rightarrow P5QLi_4$	-1.39	-2.55	-2.35	-1.58
$P5QLi_4 \rightarrow P5QLi_5$	-0.24	-2.73	-0.76	-2.2
$P5QLi_5 \rightarrow P5QLi_6$	-0.13	-2.52	-1.32	-1.33
$P5QLi_6 \rightarrow P5QLi_7$	-0.73	-2.37	-1.51	-1.58
$P5QLi_7 \rightarrow P5QLi_8$	-0.24	-2.22	-1.31	-1.15
$P5QLi_8 \rightarrow P5QLi_9$	-0.11	-2.24	-0.85	-1.5
$P5QLi_9 \rightarrow P5QLi_{10}$	-1.01	-2.05	-1.23	-1.83

Scheme S1. The example of how ion transfer step affects electron transfer step in redox reaction of C4Q.

Initial state : the activity of Li^+ ions is A_0 ($A_0 > K_{eq5}^{-1}$)

$$\Delta G_{eq4}^{o} = \Delta G_{eq4}^{\theta} + RT\ln A_0$$

$$\Delta G_{eq5}^{o} = RT\ln Q_{r0} - RT\ln K_{eq5} = RT\ln\frac{K_{eq5}^{-1}}{A_0}$$

After change: the activity of Li^+ ion changed from A_0 to a_{Li^+} by eq.5 ($A_0 > a_{Li^+} > K_{eq5}^{-1}$)

$$\Delta G_{eq4} = \Delta G_{eq4}^{\theta} + RT\ln a_{Li^+} = \Delta G_{eq4}^{o} - RT\ln A_0 + RT\ln a_{Li^+} = \Delta G_{eq4}^{o} + RT\ln\frac{a_{Li^+}}{A_0}$$

$$= \Delta G_{eq4}^{o} + \Delta G_{eq5}^{o}\left(\frac{\ln\frac{a_{Li^+}}{A_0}}{\ln\frac{K_{eq5}^{-1}}{A_0}}\right) = \Delta G_{eq4}^{o} + x\Delta G_{eq5}^{o}$$

when $a_{Li^+} \approx A_0$, $x \approx 0$

Table S5. Total energies of C4Q with different reduced forms.

Species	Total energy (hartree)
C4Q	-1678.358437
$C4Q^{1-}$	-1678.487718
$C4Q^{2-}$	-1678.598450
$C4Q^{3-}$	-1678.708953
$C4Q^{4-}$	-1678.774100
$C4Q^{5-}$	-1678.868073
$C4Q^{6-}$	-1678.903497
$C4Q^{7-}$	-1678.947915
$C4Q^{8-}$	-1678.969160
$C4Q^{9-}$	-1678.909438

Optimized geometries

C4Q

E= -1678.35843681 hartrees

Symbol	X	Y	Z
C	1.13060300	4.19445000	1.26918200
C	1.14382700	2.84800600	1.29134100
C	1.15194700	2.09191900	0.00000000
C	1.14382700	2.84800600	-1.29134100
C	1.13060300	4.19445000	-1.26918200
C	1.12651100	4.95638100	0.00000000
C	-2.42372200	0.55301600	-2.77766900
C	-1.29377000	1.50332100	-2.71917800
C	-0.01396300	1.08701800	-2.67687200
C	0.28423500	-0.38012400	-2.77815800
C	-0.85023400	-1.35128500	-2.66586900
C	-2.11490100	-0.89228700	-2.69785500
C	-0.52600400	-3.04267000	0.00000000
C	0.22464700	-3.18029800	1.28909700
C	1.48832400	-3.64272200	1.26715700
C	2.18567300	-3.95370100	0.00000000
C	1.48832400	-3.64272200	-1.26715700
C	0.22464700	-3.18029800	-1.28909700
C	0.28423500	-0.38012400	2.77815800
C	-0.01396300	1.08701800	2.67687200
C	-1.29377000	1.50332100	2.71917800
C	-2.42372200	0.55301600	2.77766900
C	-2.11490100	-0.89228700	2.69785500
C	-0.85023400	-1.35128500	2.66586900
C	1.16571300	2.03266500	2.56277800
C	-0.50601000	-2.82354700	2.56701500
C	-0.50601000	-2.82354700	-2.56701500
C	1.16571300	2.03266500	-2.56277800
O	1.15719300	0.86364900	0.00000000
O	1.42596700	-0.77749600	2.98169800
O	1.42596700	-0.77749600	-2.98169800
O	-1.73606800	-2.83877200	0.00000000
O	3.32312500	-4.42189200	0.00000000
O	-3.58615800	0.94852500	-2.85491900
O	1.11752800	6.18598900	0.00000000
O	-3.58615800	0.94852500	2.85491900
H	1.12426800	4.78282000	2.18311100

H	1.12426800	4.78282000	-2.18311100
H	-1.55634600	2.55819500	-2.69095700
H	-2.96860800	-1.56328300	-2.65702400
H	2.05942200	-3.79440000	2.17897100
H	2.05942200	-3.79440000	-2.17897100
H	-1.55634600	2.55819500	2.69095700
H	-2.96860800	-1.56328300	2.65702400
H	2.08258200	1.43552700	2.59929600
H	1.17966800	2.71585600	3.41819000
H	-1.43536300	-3.39861600	2.62683100
H	0.12591400	-3.10528500	3.41514600
H	-1.43536300	-3.39861600	-2.62683100
H	0.12591400	-3.10528500	-3.41514600
H	1.17966800	2.71585600	-3.41819000
H	2.08258200	1.43552700	-2.59929600

C4Q^{1-}

E= -1678.48771757 hartrees

Symbol	X	Y	Z
C	1.05795200	4.18067000	1.26710500
C	1.10450900	2.83359700	1.28996600
C	1.19329400	2.08160100	0.00000000
C	1.10450900	2.83359700	-1.28996600
C	1.05795200	4.18067000	-1.26710500
C	1.05656000	4.94315000	0.00000000
C	-2.47360600	0.45817700	-2.43801600
C	-1.36106100	1.42434500	-2.46942600
C	-0.07322700	1.03582800	-2.59736200
C	0.24727500	-0.40913900	-2.79430300
C	-0.84773100	-1.39933800	-2.60218900
C	-2.12336100	-0.96859900	-2.45576200
C	-0.48110000	-3.10086000	0.00000000
C	0.28673100	-3.15346100	1.26498800
C	1.62096300	-3.41554800	1.24489800
C	2.36594300	-3.60990300	0.00000000
C	1.62096300	-3.41554800	-1.24489800
C	0.28673100	-3.15346100	-1.26498800
C	0.24727500	-0.40913900	2.79430300
C	-0.07322700	1.03582800	2.59736200
C	-1.36106100	1.42434500	2.46942600
C	-2.47360600	0.45817700	2.43801600
C	-2.12336100	-0.96859900	2.45576200

C	-0.84773100	-1.39933800	2.60218900
C	1.08928500	2.01148600	2.55592700
C	-0.46509800	-2.86289600	2.54906500
C	-0.46509800	-2.86289600	-2.54906500
C	1.08928500	2.01148600	-2.55592700
O	1.33635400	0.86105600	0.00000000
O	1.37999800	-0.76570100	3.13251100
O	1.37999800	-0.76570100	-3.13251100
O	-1.72453700	-3.02714000	0.00000000
O	3.57994800	-3.89892200	0.00000000
O	-3.65044200	0.83769300	-2.36756200
O	1.03233400	6.17468100	0.00000000
O	-3.65044200	0.83769300	2.36756200
H	1.01138900	4.76774800	2.18099600
H	1.01138900	4.76774800	-2.18099600
H	-1.63310500	2.47178700	-2.35795700
H	-2.94448500	-1.66979300	-2.33744300
H	2.19359700	-3.47285400	2.16711100
H	2.19359700	-3.47285400	-2.16711100
H	-1.63310500	2.47178700	2.35795700
H	-2.94448500	-1.66979300	2.33744300
H	2.01410300	1.43077100	2.63469600
H	1.04941500	2.68831000	3.41661400
H	-1.37512800	-3.46854000	2.59984600
H	0.17148800	-3.11476900	3.40298800
H	-1.37512800	-3.46854000	-2.59984600
H	0.17148800	-3.11476900	-3.40298800
H	1.04941500	2.68831000	-3.41661400
H	2.01410300	1.43077100	-2.63469600

$C4Q^{2-}$

E= -1678.59845045 hartrees

Symbol	X	Y	Z
C	1.04145600	4.19947000	1.25000000
C	1.05212400	2.84024800	1.26898700
C	1.13771400	2.08651500	0.00000000
C	1.05212400	2.84024800	-1.26898700
C	1.04145600	4.19947000	-1.25000000
C	1.05572700	4.96809000	0.00000000
C	-2.50128200	0.39461100	-2.28988400
C	-1.41019900	1.37425200	-2.36695200
C	-0.11511300	1.01241800	-2.55510100

C	0.23578000	-0.41046500	-2.77271400
C	-0.83039100	-1.41445900	-2.55243600
C	-2.11555800	-1.01491000	-2.34156700
C	-0.42276800	-3.14668200	0.00000000
C	0.34861300	-3.14186800	1.26134700
C	1.70072300	-3.31315200	1.24149700
C	2.45871400	-3.46239300	0.00000000
C	1.70072300	-3.31315200	-1.24149700
C	0.34861300	-3.14186800	-1.26134700
C	0.23578000	-0.41046500	2.77271400
C	-0.11511300	1.01241800	2.55510100
C	-1.41019900	1.37425200	2.36695200
C	-2.50128200	0.39461100	2.28988400
C	-2.11555800	-1.01491000	2.34156700
C	-0.83039100	-1.41445900	2.55243600
C	1.01649100	2.02388200	2.54151400
C	-0.41910500	-2.87148000	2.53887800
C	-0.41910500	-2.87148000	-2.53887800
C	1.01649100	2.02388200	-2.54151400
O	1.28075800	0.84921400	0.00000000
O	1.37215500	-0.74559600	3.15407200
O	1.37215500	-0.74559600	-3.15407200
O	-1.67097500	-3.16977800	0.00000000
O	3.69025700	-3.68139200	0.00000000
O	-3.68923400	0.75126800	-2.16300000
O	1.04161700	6.21367300	0.00000000
O	-3.68923400	0.75126800	2.16300000
H	1.00070200	4.77663000	2.17170800
H	1.00070200	4.77663000	-2.17170800
H	-1.69145100	2.41726200	-2.23265300
H	-2.91045200	-1.74298200	-2.20525300
H	2.27273900	-3.32585800	2.16572500
H	2.27273900	-3.32585800	-2.16572500
H	-1.69145100	2.41726200	2.23265300
H	-2.91045200	-1.74298200	2.20525300
H	1.95151900	1.46441800	2.65788500
H	0.93254700	2.70573900	3.39685200
H	-1.31295700	-3.50129800	2.58754100
H	0.21796100	-3.09403000	3.40063300
H	-1.31295700	-3.50129800	-2.58754100
H	0.21796100	-3.09403000	-3.40063300
H	0.93254700	2.70573900	-3.39685200
H	1.95151900	1.46441800	-2.65788500

$C4Q^{3-}$

E= -1678.70895276 hartrees

Symbol	X	Y	Z
C	1.04862500	4.17801600	1.22730000
C	1.10394100	2.80347700	1.24495400
C	1.17492100	2.04578400	0.00000000
C	1.10394100	2.80347700	-1.24495400
C	1.04862500	4.17801600	-1.22730000
C	1.03739800	4.95330500	0.00000000
C	-2.47768100	0.43505700	-2.34376500
C	-1.36845800	1.38912000	-2.40917600
C	-0.07317700	1.00864600	-2.57735500
C	0.25081800	-0.42199300	-2.80706600
C	-0.83182300	-1.40256400	-2.58364200
C	-2.11325400	-0.97659200	-2.37500700
C	-0.47950800	-3.09522200	0.00000000
C	0.29528400	-3.13112100	1.25130200
C	1.65119200	-3.33645700	1.22995700
C	2.41167000	-3.49776600	0.00000000
C	1.65119200	-3.33645700	-1.22995700
C	0.29528400	-3.13112100	-1.25130200
C	0.25081800	-0.42199300	2.80706600
C	-0.07317700	1.00864600	2.57735500
C	-1.36845800	1.38912000	2.40917600
C	-2.47768100	0.43505700	2.34376500
C	-2.11325400	-0.97659200	2.37500700
C	-0.83182300	-1.40256400	2.58364200
C	1.07670600	2.00014800	2.53215000
C	-0.45275400	-2.86678300	2.54274400
C	-0.45275400	-2.86678300	-2.54274400
C	1.07670600	2.00014800	-2.53215000
O	1.26745500	0.78238600	0.00000000
O	1.37882900	-0.77626100	3.20310100
O	1.37882900	-0.77626100	-3.20310100
O	-1.73670100	-3.05962300	0.00000000
O	3.64609300	-3.75182400	0.00000000
O	-3.66654900	0.81556700	-2.24725300
O	0.99877000	6.22046000	0.00000000
O	-3.66654900	0.81556700	2.24725300
H	1.00034400	4.74101700	2.15985600
H	1.00034400	4.74101700	-2.15985600
H	-1.62988000	2.43757500	-2.27139300

H	-2.91856100	-1.69266100	-2.23515400
H	2.21348600	-3.37611900	2.16049700
H	2.21348600	-3.37611900	-2.16049700
H	-1.62988000	2.43757500	2.27139300
H	-2.91856100	-1.69266100	2.23515400
H	2.00035100	1.42276100	2.64779100
H	1.01626200	2.69152800	3.38361000
H	-1.36086700	-3.47724500	2.59272600
H	0.18819600	-3.11893200	3.39439300
H	-1.36086700	-3.47724500	-2.59272600
H	0.18819600	-3.11893200	-3.39439300
H	1.01626200	2.69152800	-3.38361000
H	2.00035100	1.42276100	-2.64779100

$C4Q^{4-}$

E= -1678.77409958 hartrees

Symbol	X	Y	Z
C	1.06051300	4.23646000	1.21206800
C	1.08314500	2.84397400	1.22492200
C	1.15426000	2.08441700	0.00000000
C	1.08314500	2.84397400	-1.22492200
C	1.06051300	4.23646000	-1.21206800
C	1.06559200	5.02573900	0.00000000
C	-2.48265100	0.43191000	-2.32506700
C	-1.38063100	1.38755900	-2.38654100
C	-0.07705400	1.01274300	-2.54165000
C	0.25849400	-0.40860000	-2.77572000
C	-0.81801900	-1.39672300	-2.54673000
C	-2.10406300	-0.97602900	-2.34431600
C	-0.48387600	-3.15578400	0.00000000
C	0.29542100	-3.17537000	1.23852700
C	1.65726900	-3.40088100	1.21863900
C	2.41970500	-3.58189400	0.00000000
C	1.65726900	-3.40088100	-1.21863900
C	0.29542100	-3.17537000	-1.23852700
C	0.25849400	-0.40860000	2.77572000
C	-0.07705400	1.01274300	2.54165000
C	-1.38063100	1.38755900	2.38654100
C	-2.48265100	0.43191000	2.32506700
C	-2.10406300	-0.97602900	2.34431600
C	-0.81801900	-1.39672300	2.54673000
C	1.04947300	2.03318300	2.51138800

C	-0.44060100	-2.86415300	2.52790600
C	-0.44060100	-2.86415300	-2.52790600
C	1.04947300	2.03318300	-2.51138800
O	1.25324100	0.80242600	0.00000000
O	1.38435500	-0.76089500	3.19233200
O	1.38435500	-0.76089500	-3.19233200
O	-1.75227000	-3.13180300	0.00000000
O	3.66149800	-3.85383300	0.00000000
O	-3.68055400	0.80038700	-2.24526800
O	1.04280200	6.30658600	0.00000000
O	-3.68055400	0.80038700	2.24526800
H	1.01709400	4.78722900	2.15506900
H	1.01709400	4.78722900	-2.15506900
H	-1.64535100	2.43686200	-2.25815600
H	-2.90410500	-1.69858400	-2.20448200
H	2.21552800	-3.42671700	2.15382200
H	2.21552800	-3.42671700	-2.15382200
H	-1.64535100	2.43686200	2.25815600
H	-2.90410500	-1.69858400	2.20448200
H	1.98225800	1.47265500	2.64784900
H	0.95628900	2.71975500	3.36622900
H	-1.35252800	-3.46785900	2.60390600
H	0.20449900	-3.09464600	3.38350600
H	-1.35252800	-3.46785900	-2.60390600
H	0.20449900	-3.09464600	-3.38350600
H	0.95628900	2.71975500	-3.36622900
H	1.98225800	1.47265500	-2.64784900

C4Q^{5-}

E= -1678.86807324 hartrees

Symbol	X	Y	Z
C	1.09027700	4.13518700	1.19935600
C	1.15464400	2.73066400	1.21758400
C	1.21039200	1.95836900	0.00000000
C	1.15464400	2.73066400	-1.21758400
C	1.09027700	4.13518700	-1.19935600
C	1.06691000	4.93378500	0.00000000
C	-2.43646100	0.56689700	-2.72350600
C	-1.28387900	1.44739200	-2.70043000
C	0.01705700	0.99708900	-2.72292300
C	0.29625100	-0.42934200	-2.91481300
C	-0.83489600	-1.33760200	-2.71958700

C	-2.12133200	-0.84559400	-2.66368700
C	-0.59107300	-3.03486300	0.00000000
C	0.17334700	-3.12810100	1.24665300
C	1.50885100	-3.45988100	1.22292800
C	2.25280700	-3.68218800	0.00000000
C	1.50885100	-3.45988100	-1.22292800
C	0.17334700	-3.12810100	-1.24665300
C	0.29625100	-0.42934200	2.91481300
C	0.01705700	0.99708900	2.72292300
C	-1.28387900	1.44739200	2.70043000
C	-2.43646100	0.56689700	2.72350600
C	-2.12133200	-0.84559400	2.66368700
C	-0.83489600	-1.33760200	2.71958700
C	1.19071200	1.95090700	2.52874700
C	-0.54081100	-2.82163300	2.55622500
C	-0.54081100	-2.82163300	-2.55622500
C	1.19071200	1.95090700	-2.52874700
O	1.30325800	0.66959300	0.00000000
O	1.44236100	-0.85811200	3.24560200
O	1.44236100	-0.85811200	-3.24560200
O	-1.85021600	-2.89610900	0.00000000
O	3.47801500	-4.02085200	0.00000000
O	-3.63272100	1.00011200	-2.74129800
O	1.02224700	6.22658800	0.00000000
O	-3.63272100	1.00011200	2.74129800
H	1.06186900	4.67968500	2.15014600
H	1.06186900	4.67968500	-2.15014600
H	-1.49097800	2.51396800	-2.59300300
H	-2.96267600	-1.52861100	-2.54643000
H	2.06714900	-3.53111900	2.15530500
H	2.06714900	-3.53111900	-2.15530500
H	-1.49097800	2.51396800	2.59300300
H	-2.96267600	-1.52861100	2.54643000
H	2.09198100	1.32742100	2.58205600
H	1.24086200	2.66534500	3.36734000
H	-1.48809300	-3.37366600	2.59426300
H	0.08987400	-3.16711800	3.38517800
H	-1.48809300	-3.37366600	-2.59426300
H	0.08987400	-3.16711800	-3.38517800
H	1.24086200	2.66534500	-3.36734000
H	2.09198100	1.32742100	-2.58205600

$C4Q^{6-}$

E= -1678.90349737 hartrees

Symbol	X	Y	Z
C	1.05965800	4.10616700	1.20492000
C	1.21126800	2.71247500	1.22533600
C	1.36660400	1.95992100	0.00000000
C	1.21126800	2.71247500	-1.22533600
C	1.05965800	4.10616700	-1.20492000
C	0.98876500	4.89757700	0.00000000
C	-2.43236800	0.59442600	-2.66735200
C	-1.25748700	1.44392500	-2.64846900
C	0.04434500	0.96989900	-2.71007300
C	0.31570300	-0.45102600	-2.90666800
C	-0.83163300	-1.32941500	-2.71448800
C	-2.12436700	-0.81148800	-2.63634300
C	-0.67061700	-3.01935500	0.00000000
C	0.10278600	-3.12607700	1.23699600
C	1.45449100	-3.44816700	1.21124800
C	2.21218400	-3.65518800	0.00000000
C	1.45449100	-3.44816700	-1.21124800
C	0.10278600	-3.12607700	-1.23699600
C	0.31570300	-0.45102600	2.90666800
C	0.04434500	0.96989900	2.71007300
C	-1.25748700	1.44392500	2.64846900
C	-2.43236800	0.59442600	2.66735200
C	-2.12436700	-0.81148800	2.63634300
C	-0.83163300	-1.32941500	2.71448800
C	1.23402000	1.91563900	2.52482500
C	-0.58519000	-2.82215500	2.55924700
C	-0.58519000	-2.82215500	-2.55924700
C	1.23402000	1.91563900	-2.52482500
O	1.61763800	0.69916100	0.00000000
O	1.47302100	-0.88922600	3.23192200
O	1.47302100	-0.88922600	-3.23192200
O	-1.93616100	-2.87229100	0.00000000
O	3.44771300	-3.99164000	0.00000000
O	-3.62773000	1.05908200	-2.67019400
O	0.84891200	6.18115100	0.00000000
O	-3.62773000	1.05908200	2.67019400
H	0.96938000	4.65161500	2.15113700
H	0.96938000	4.65161500	-2.15113700
H	-1.43638100	2.51565300	-2.52366800
H	-2.96844800	-1.49518500	-2.52922500
H	2.00191900	-3.52167000	2.15122300

H	2.00191900	-3.52167000	-2.15122300
H	-1.43638100	2.51565300	2.52366800
H	-2.96844800	-1.49518500	2.52922500
H	2.11982900	1.27001700	2.56410000
H	1.30192100	2.62074600	3.37258200
H	-1.54857200	-3.34845000	2.61184400
H	0.04745400	-3.19119400	3.37969800
H	-1.54857200	-3.34845000	-2.61184400
H	0.04745400	-3.19119400	-3.37969800
H	1.30192100	2.62074600	-3.37258200
H	2.11982900	1.27001700	-2.56410000

C4Q^{7-}

E= -1678.94791468 hartrees

Symbol	X	Y	Z
C	1.06660500	4.04501200	1.19640700
C	1.31268000	2.65601900	1.22047700
C	1.50400800	1.90170700	0.00000000
C	1.31268000	2.65601900	-1.22047700
C	1.06660500	4.04501200	-1.19640700
C	0.94827300	4.83790400	0.00000000
C	-2.35917100	0.74053800	-2.88337100
C	-1.14816200	1.51948700	-2.80448700
C	0.14263800	0.98197100	-2.79489800
C	0.35833400	-0.44874300	-2.96059000
C	-0.83537400	-1.25837100	-2.78509500
C	-2.11130900	-0.67276900	-2.79881700
C	-0.81008900	-2.98816300	0.00000000
C	-0.04347400	-3.13509700	1.23448100
C	1.27617400	-3.58250100	1.20498000
C	2.00473900	-3.88692900	0.00000000
C	1.27617400	-3.58250100	-1.20498000
C	-0.04347400	-3.13509700	-1.23448100
C	0.35833400	-0.44874300	2.96059000
C	0.14263800	0.98197100	2.79489800
C	-1.14816200	1.51948700	2.80448700
C	-2.35917100	0.74053800	2.88337100
C	-2.11130900	-0.67276900	2.79881700
C	-0.83537400	-1.25837100	2.78509500
C	1.36336400	1.87246700	2.53140600
C	-0.68580600	-2.76274900	2.56942500
C	-0.68580600	-2.76274900	-2.56942500

C	1.36336400	1.87246700	-2.53140600
O	1.81127200	0.64991500	0.00000000
O	1.51167500	-0.94787000	3.24329200
O	1.51167500	-0.94787000	-3.24329200
O	-2.06642000	-2.73767700	0.00000000
O	3.19777700	-4.37097800	0.00000000
O	-3.53922300	1.26043600	-2.97696900
O	0.75029800	6.12255700	0.00000000
O	-3.53922300	1.26043600	2.97696900
H	0.95817900	4.58340200	2.14750400
H	0.95817900	4.58340200	-2.14750400
H	-1.27350000	2.60360900	-2.70772500
H	-2.99114300	-1.31733700	-2.70862900
H	1.81695700	-3.69485500	2.14642700
H	1.81695700	-3.69485500	-2.14642700
H	-1.27350000	2.60360900	2.70772500
H	-2.99114300	-1.31733700	2.70862900
H	2.21446100	1.18101500	2.52284300
H	1.51712300	2.58263900	3.36749400
H	-1.68303700	-3.22379500	2.63445400
H	-0.07015600	-3.19561300	3.37387500
H	-1.68303700	-3.22379500	-2.63445400
H	-0.07015600	-3.19561300	-3.37387500
H	1.51712300	2.58263900	-3.36749400
H	2.21446100	1.18101500	-2.52284300

C4Q^{8-}

E= -1678.96916033 hartrees

Symbol	X	Y	Z
C	1.14348400	4.15433300	1.19509800
C	1.10108900	2.74313700	1.22478100
C	1.08402200	1.96458500	0.00000000
C	1.10108900	2.74313700	-1.22478100
C	1.14348400	4.15433300	-1.19509800
C	1.15832400	4.95642700	0.00000000
C	-2.41175100	0.61079300	-3.20440500
C	-1.27015600	1.47085100	-3.03672300
C	0.05575900	1.02079400	-2.90847900
C	0.40038200	-0.38396100	-3.04012600
C	-0.73622100	-1.27425600	-2.94167600
C	-2.05367900	-0.77614000	-3.08418800
C	-0.69868500	-2.94939900	0.00000000

C	0.07785000	-3.11427900	1.22423300
C	1.37421800	-3.67051000	1.18822600
C	2.08947100	-4.03743800	0.00000000
C	1.37421800	-3.67051000	-1.18822600
C	0.07785000	-3.11427900	-1.22423300
C	0.40038200	-0.38396100	3.04012600
C	0.05575900	1.02079400	2.90847900
C	-1.27015600	1.47085100	3.03672300
C	-2.41175100	0.61079300	3.20440500
C	-2.05367900	-0.77614000	3.08418800
C	-0.73622100	-1.27425600	2.94167600
C	1.19305400	1.98382800	2.55531800
C	-0.52779600	-2.75956700	2.59827400
C	-0.52779600	-2.75956700	-2.59827400
C	1.19305400	1.98382800	-2.55531800
O	1.08584600	0.68026100	0.00000000
O	1.61956000	-0.79078900	3.19828100
O	1.61956000	-0.79078900	-3.19828100
O	-1.96350200	-2.66849900	0.00000000
O	3.25970000	-4.61041000	0.00000000
O	-3.62593100	1.04206300	-3.39055800
O	1.19772400	6.25738900	0.00000000
O	-3.62593100	1.04206300	3.39055800
H	1.18087600	4.70168400	2.14729700
H	1.18087600	4.70168400	-2.14729700
H	-1.47480800	2.54761400	-2.95944200
H	-2.88740800	-1.48925000	-3.04231700
H	1.90032400	-3.82799500	2.13763100
H	1.90032400	-3.82799500	-2.13763100
H	-1.47480800	2.54761400	2.95944200
H	-2.88740800	-1.48925000	3.04231700
H	2.08252600	1.33658200	2.56078200
H	1.34343900	2.73321200	3.35915100
H	-1.51136600	-3.25304900	2.68527800
H	0.12152300	-3.22662300	3.36015400
H	-1.51136600	-3.25304900	-2.68527800
H	0.12152300	-3.22662300	-3.36015400
H	1.34343900	2.73321200	-3.35915100
H	2.08252600	1.33658200	-2.56078200

$C4Q^{9-}$

E= -1678.90943820 hartrees

Symbol	X	Y	Z
C	0.90762900	3.87621300	1.20212800
C	1.57090600	2.58035000	1.23644100
C	2.02130200	1.95268200	0.00000000
C	1.57090600	2.58035000	-1.23644100
C	0.90762900	3.87621300	-1.20212800
C	0.60616000	4.60753200	0.00000000
C	-2.14255200	0.99040700	-3.36446700
C	-0.87189400	1.65184700	-3.21700200
C	0.36272900	1.00422800	-2.95269300
C	0.43489800	-0.45535200	-3.00657400
C	-0.84246500	-1.12228900	-2.88646000
C	-2.05465700	-0.41897200	-3.11431200
C	-1.01870400	-2.74755100	0.00000000
C	-0.31730700	-3.09529100	1.22228100
C	0.82327500	-3.92439100	1.19080900
C	1.43978300	-4.43854900	0.00000000
C	0.82327500	-3.92439100	-1.19080900
C	-0.31730700	-3.09529100	-1.22228100
C	0.43489800	-0.45535200	3.00657400
C	0.36272900	1.00422800	2.95269300
C	-0.87189400	1.65184700	3.21700200
C	-2.14255200	0.99040700	3.36446700
C	-2.05465700	-0.41897200	3.11431200
C	-0.84246500	-1.12228900	2.88646000
C	1.63451500	1.78782000	2.54799100
C	-0.88318400	-2.62379200	2.57029000
C	-0.88318400	-2.62379200	-2.57029000
C	1.63451500	1.78782000	-2.54799100
O	2.77836500	0.89446500	0.00000000
O	1.54894200	-1.10667200	3.14511700
O	1.54894200	-1.10667200	-3.14511700
O	-2.19554600	-2.20652100	0.00000000
O	2.45487400	-5.25669900	0.00000000
O	-3.24965000	1.61092900	-3.66665800
O	0.10099400	5.81539400	0.00000000
O	-3.24965000	1.61092900	3.66665800
H	0.72117900	4.40447100	2.15224000
H	0.72117900	4.40447100	-2.15224000
H	-0.90498200	2.74759500	-3.25455100
H	-3.00220400	-0.97414800	-3.07669100
H	1.29560500	-4.20455700	2.14070300
H	1.29560500	-4.20455700	-2.14070300
H	-0.90498200	2.74759500	3.25455100

H	-3.00220400	-0.97414800	3.07669100
H	2.41467800	1.02420300	2.45119400
H	1.94099600	2.47616100	3.38948300
H	-1.94137400	-2.93640900	2.62692100
H	-0.34996400	-3.18493400	3.36126000
H	-1.94137400	-2.93640900	-2.62692100
H	-0.34996400	-3.18493400	-3.36126000
H	1.94099600	2.47616100	-3.38948300
H	2.41467800	1.02420300	-2.45119400

$C4QLi_1$ (by condensed Fukui function)

E= -1686.127594 hartrees

Symbol	X	Y	Z
C	-4.24635100	1.27014400	-1.11311300
C	-2.89964100	1.29262800	-1.17287100
C	-2.16113200	-0.00006100	-1.34458000
C	-2.89930900	-1.29293900	-1.17287100
C	-4.24603000	-1.27076300	-1.11312200
C	-5.00486600	-0.00041000	-1.14348600
C	-0.43857500	-1.92920000	2.37126100
C	-1.41983100	-2.12605800	1.31762800
C	-1.05723900	-2.47312600	0.05262300
C	0.36933600	-2.74920600	-0.25612300
C	1.37418200	-2.48044100	0.80254600
C	0.96445000	-2.13070500	2.05306000
C	3.25818500	0.00014900	0.43253000
C	3.22831800	1.28808200	-0.33195400
C	3.53619500	1.26654800	-1.64554000
C	3.79454600	-0.00013800	-2.36206900
C	3.53643300	-1.26668300	-1.64523800
C	3.22853900	-1.28796800	-0.33164500
C	0.36886100	2.74934200	-0.25638600
C	-1.05775400	2.47315600	0.05248600
C	-1.42016400	2.12621800	1.31751700
C	-0.43869500	1.92945500	2.37105400
C	0.96436800	2.13104100	2.05273400
C	1.37394300	2.48064200	0.80219800
C	-2.06490100	2.54791400	-1.08202700
C	2.84268300	2.54343700	0.42502200
C	2.84299700	-2.54317900	0.42559600
C	-2.06429400	-2.54802900	-1.08198200
O	-0.96449400	0.00011900	-1.62012400

O	0.71016300	3.20458000	-1.36117800
O	0.71082400	-3.20439100	-1.36097500
O	3.33294200	0.00031700	1.66028400
O	4.16441400	-0.00023000	-3.54194600
O	-0.79416500	-1.53697400	3.52219100
O	-6.23932000	-0.00055900	-1.14571700
O	-0.79409400	1.53721400	3.52192200
H	-4.83192300	2.18230900	-1.02288800
H	-4.83138000	-2.18307000	-1.02289200
H	-2.45835700	-1.92790000	1.57381800
H	1.68303300	-1.94051200	2.84542400
H	3.58581000	2.17737900	-2.23692200
H	3.58620100	-2.17764900	-2.23639700
H	-2.45863100	1.92801400	1.57389800
H	1.68299000	1.94094000	2.84507900
H	-1.51561200	2.70217100	-2.01653400
H	-2.73206700	3.40730700	-0.94715100
H	3.44289000	2.62845500	1.33628100
H	3.03802700	3.41338700	-0.20774000
H	3.44310600	-2.62788700	1.33695000
H	3.03854600	-3.41325700	-0.20693000
H	-2.73129800	-3.40757500	-0.94726000
H	-1.51485300	-2.70211100	-2.01643200
Li	-1.00738500	0.00009700	4.47152000

$C4QLi_2$ (by condensed Fukui function)

E= -1693.744103 hartrees

Symbol	X	Y	Z
C	-4.13099200	1.35425900	-0.59656500
C	-2.80945300	1.34965000	-0.86486700
C	-2.17302400	0.05615000	-1.27045200
C	-2.87836300	-1.22349700	-0.95293700
C	-4.19884500	-1.17462800	-0.67689900
C	-4.92746500	0.10689200	-0.57768000
C	-0.07715500	-2.13174900	2.35546100
C	-1.15046800	-2.24798700	1.40246700
C	-0.91840800	-2.42626900	0.05702100
C	0.44246000	-2.50914100	-0.45035000
C	1.52939200	-2.50614300	0.51678900
C	1.25328800	-2.31417900	1.86152000
C	3.35303700	-0.00928400	0.13677900
C	3.11839800	1.30848500	-0.53373700

C	2.81897200	1.35361200	-1.85998500
C	2.57615600	0.12169500	-2.60309100
C	2.99045000	-1.13754700	-2.01438600
C	3.19429100	-1.24147100	-0.67182500
C	0.49863400	2.85217700	-0.02120900
C	-0.88529800	2.42919000	0.31364400
C	-1.14555500	1.92167100	1.54674800
C	-0.08498400	1.69063900	2.52559000
C	1.28911300	1.96718700	2.13684300
C	1.59420000	2.47068000	0.90907000
C	-1.93782200	2.57485700	-0.77412000
C	3.00730900	2.52784200	0.36355900
C	2.97583900	-2.55864200	0.03294900
C	-2.06849500	-2.49359000	-0.94161600
O	-1.09173000	0.05561400	-1.87365300
O	0.73015400	3.49955700	-1.05263600
O	0.65724900	-2.56077700	-1.72021600
O	3.68070700	-0.06011900	1.33097900
O	1.84291900	0.11146500	-3.63458900
O	-0.31557000	-1.86831900	3.59831900
O	-6.15025100	0.13685300	-0.41841700
O	-0.35630700	1.20483200	3.65815400
H	-4.65955500	2.27390400	-0.35685900
H	-4.77448700	-2.07897000	-0.49348200
H	-2.16734700	-2.15747300	1.78102400
H	2.06795700	-2.26694000	2.58012900
H	2.57508100	2.29119600	-2.35081200
H	2.87952400	-2.02516400	-2.62702300
H	-2.14952000	1.62478800	1.84100500
H	2.06802800	1.69705500	2.84414300
H	-1.42565700	2.75569100	-1.72384900
H	-2.57094500	3.44839300	-0.57806000
H	3.72993400	2.48270500	1.18141000
H	3.16791700	3.43966500	-0.21734600
H	3.64462500	-2.68887300	0.88787700
H	3.13164500	-3.38416900	-0.66951900
H	-2.73814800	-3.32439700	-0.69349300
H	-1.65772900	-2.69342900	-1.93689600
Li	-0.53398000	-0.37918800	4.55753200
Li	0.32399700	-1.02481400	-2.77890000

C_4QLi_3 (by condensed Fukui function)

E= -1701.357884 hartrees

Symbol	X	Y	Z
C	-4.32615500	0.50116200	-0.85666700
C	-3.02441600	0.65283100	-1.17884900
C	-2.14981300	-0.56567900	-1.17536000
C	-2.60137200	-1.77501100	-0.42016500
C	-3.90591800	-1.87216800	-0.08823600
C	-4.86669500	-0.78471300	-0.36998800
C	0.57451800	-1.32118300	2.70504400
C	-0.55673500	-1.73712600	1.93129300
C	-0.39442200	-2.36109000	0.70916800
C	0.93666100	-2.54662000	0.14449100
C	2.06190200	-2.28647900	1.00616500
C	1.84403100	-1.76776200	2.28335200
C	3.11035800	0.33688100	0.07352300
C	2.74907100	1.43023900	-0.86751300
C	2.52471400	1.13919800	-2.17765200
C	2.51149800	-0.24788800	-2.63509500
C	3.15448100	-1.23894600	-1.80452100
C	3.36718400	-1.00804700	-0.47121700
C	-0.05130800	2.75366100	-0.85004800
C	-1.39018100	2.36132500	-0.41549300
C	-1.68345500	2.26825300	0.92444200
C	-0.68588100	2.46360000	1.94433000
C	0.66003100	2.72144100	1.50728600
C	0.99593300	2.80101900	0.17279700
C	-2.39957000	1.98674100	-1.49477500
C	2.43952100	2.80900800	-0.30228200
C	3.47305900	-2.20659100	0.45059500
C	-1.58610600	-2.84202500	-0.11092300
O	-1.08634400	-0.57848200	-1.80878600
O	0.19493000	3.02173900	-2.05969000
O	1.07848100	-2.88621800	-1.09822900
O	3.17837500	0.57789300	1.30982400
O	1.81693100	-0.60098200	-3.63339200
O	0.49525100	-0.44604100	3.69814100
O	-6.07171700	-0.92746100	-0.14522400
O	-0.97271600	2.31748800	3.19600000
H	-5.02167800	1.33605700	-0.89963200
H	-4.30292200	-2.75656500	0.40478500
H	-1.55389800	-1.51144300	2.30729200
H	2.70255000	-1.56655000	2.92368500
H	2.17073300	1.90122100	-2.86359300
H	3.27165500	-2.23495000	-2.21661200

H	-2.67939100	1.98394000	1.25851000
H	1.42674200	2.84442700	2.27454800
H	-1.87199300	1.95821500	-2.45293700
H	-3.19376900	2.73839100	-1.57606400
H	3.10623500	3.04530800	0.53122900
H	2.57755000	3.55505800	-1.09067000
H	4.19165600	-2.06655200	1.26337500
H	3.76186700	-3.08749500	-0.13022500
H	-2.09636800	-3.65243500	0.42304900
H	-1.20408400	-3.26958900	-1.04456400
Li	-0.75397800	0.80333700	4.16462600
Li	0.48162500	-1.69311200	-2.44050700
Li	1.92701500	0.54820700	2.74803500

$C4QLi_4$ (by condensed Fukui function)

E= -1708.977769 hartrees

Symbol	X	Y	Z
C	-4.29867000	0.41473500	-0.83629800
C	-2.99464100	0.45262200	-1.19934000
C	-2.16084700	-0.76365900	-0.96451200
C	-2.64897400	-1.77356100	0.01840900
C	-3.95880400	-1.77094200	0.35294500
C	-4.88786500	-0.73444800	-0.13125600
C	0.47026000	-0.51768100	2.88701700
C	-0.65735200	-1.13326100	2.25890900
C	-0.49049700	-2.12592500	1.30682300
C	0.83487400	-2.53291900	0.88495700
C	1.95391000	-2.00784500	1.61966100
C	1.73442900	-1.09658900	2.65552300
C	3.14231200	0.24558300	0.00852000
C	2.88151900	1.05137500	-1.18868000
C	2.61757600	0.42182400	-2.38052500
C	2.36854900	-0.99421500	-2.39247800
C	2.97543500	-1.78960100	-1.36645300
C	3.28161300	-1.21558000	-0.15199700
C	0.08934100	2.19955100	-1.41396500
C	-1.25518800	2.22127300	-0.88211700
C	-1.50197900	2.68156300	0.39840200
C	-0.44991800	3.10738900	1.27312000
C	0.87437600	3.09063800	0.73463800
C	1.15983200	2.65570300	-0.56354600
C	-2.37299700	1.69685100	-1.77681900

C	2.59922500	2.53442700	-1.05118300
C	3.36515600	-2.11979300	1.06345000
C	-1.67852300	-2.76562300	0.60163900
O	-1.08867400	-0.95706700	-1.58812600
O	0.30093200	1.75872900	-2.61768000
O	0.98454500	-3.29030300	-0.16396100
O	3.23740800	0.80072900	1.14777200
O	1.45668300	-1.49228000	-3.17138100
O	0.39648800	0.64038500	3.53295900
O	-6.09994200	-0.79499400	0.10603000
O	-0.69695900	3.46525100	2.50640900
H	-4.95885300	1.25506400	-1.03710800
H	-4.36924500	-2.52546900	1.01982000
H	-1.65063400	-0.75438500	2.49558600
H	2.59108300	-0.69825500	3.19617200
H	2.38197000	0.99615100	-3.26786600
H	2.97622000	-2.86796000	-1.47773500
H	-2.51835000	2.69588100	0.79037600
H	1.68051400	3.48504400	1.35746200
H	-1.96728600	1.51103300	-2.77624500
H	-3.16266600	2.44802300	-1.88642700
H	3.27393900	3.01412700	-0.33633900
H	2.72432600	3.01899500	-2.02649500
H	4.09343300	-1.77378700	1.80269800
H	3.62710600	-3.13534700	0.75180300
H	-2.23259700	-3.40068700	1.30339000
H	-1.29666200	-3.43196100	-0.17956900
Li	-0.67174900	2.10187900	3.69405100
Li	0.42913700	-2.52871800	-1.77409200
Li	1.83058000	1.29825700	2.32900000
Li	0.05568000	-0.02855500	-3.02721700

$C4QLi_5$ (by condensed Fukui function)

E= -1716.593386 hartrees

Symbol	X	Y	Z
C	-4.28412600	0.20534300	-0.87474700
C	-2.98924000	0.30712100	-1.30047600
C	-2.07064000	-0.83308300	-1.09772300
C	-2.50173600	-1.89479200	-0.16399400
C	-3.80394900	-1.95650100	0.23001000
C	-4.79620100	-0.95898100	-0.16627200
C	0.37632800	-0.59844200	2.87358900

C	-0.65949800	-1.25728900	2.16852200
C	-0.37246400	-2.20948500	1.18007800
C	0.97359400	-2.50061500	0.82422500
C	2.01523100	-1.90591600	1.58348600
C	1.68714700	-1.06485600	2.65485000
C	3.13694900	0.56598400	0.12556900
C	2.83391400	1.39642400	-1.03202700
C	2.67066600	0.81432500	-2.26980600
C	2.55439300	-0.60654100	-2.37188700
C	3.17217400	-1.39545100	-1.35419900
C	3.38072300	-0.86293400	-0.09769900
C	-0.10323200	2.31305300	-1.33960800
C	-1.46878300	2.21765200	-0.87581000
C	-1.80869200	2.60597900	0.41361600
C	-0.83181600	3.05575000	1.34754500
C	0.51462100	3.18085200	0.86243200
C	0.89595600	2.82215700	-0.42674200
C	-2.48475600	1.62155400	-1.84334400
C	2.36812700	2.83190300	-0.83916300
C	3.45302400	-1.83707400	1.07131000
C	-1.49180800	-2.87360200	0.38294200
O	-0.95403800	-0.92857300	-1.71317700
O	0.19767900	1.91191700	-2.53455300
O	1.22611100	-3.25015200	-0.27456600
O	3.13965500	1.07428400	1.30500700
O	1.68840300	-1.14473800	-3.19399900
O	0.20578500	0.52651900	3.58617200
O	-6.00392700	-1.07747800	0.13683100
O	-1.12824500	3.29903000	2.59914200
H	-4.98082500	1.02303100	-1.04521500
H	-4.14317400	-2.75455900	0.88698500
H	-1.69080100	-0.95733000	2.34828700
H	2.49755600	-0.61852700	3.22989300
H	2.36603800	1.41864300	-3.11534800
H	3.23702700	-2.46768500	-1.50671100
H	-2.83794400	2.51738500	0.75944600
H	1.26141800	3.57676600	1.55398800
H	-2.01386400	1.50977200	-2.82413500
H	-3.34203700	2.29226900	-1.97045800
H	2.95308600	3.34483000	-0.06989500
H	2.49400000	3.37431600	-1.78419800
H	4.11280600	-1.48264600	1.86898900
H	3.82854700	-2.80336100	0.71758600
H	-2.02901800	-3.58711800	1.02056600

H	-1.04602400	-3.46438300	-0.42374800
Li	-0.97252300	1.88272300	3.71902400
Li	0.65140200	-2.20667900	-1.76903800
Li	1.63287600	1.28512700	2.42890100
Li	0.11334900	0.12542700	-3.01834000
Li	1.96370000	-4.85428900	-0.33419900

$C4QLi_6$ (by condensed Fukui function)

E= -1724.210611 hartrees

Symbol	X	Y	Z
C	-4.11733700	0.56889400	-0.98983200
C	-2.76708000	0.57521200	-1.37242500
C	-1.96266300	-0.59171000	-1.23525400
C	-2.52592700	-1.66553700	-0.48928000
C	-3.87902800	-1.64312800	-0.11222200
C	-4.73778100	-0.55428300	-0.39254000
C	0.24099800	-0.97122400	2.83554900
C	-0.79652000	-1.49591200	2.02564300
C	-0.52423700	-2.33610000	0.93972700
C	0.82523900	-2.65762700	0.60800200
C	1.86380000	-2.19769600	1.45890800
C	1.53904400	-1.46436000	2.60768100
C	3.15288000	0.37493100	0.27999700
C	3.03468000	1.34455600	-0.80507500
C	2.89282100	0.90510500	-2.10713100
C	2.65935000	-0.48561900	-2.35974800
C	3.15927200	-1.43002300	-1.38767100
C	3.31437700	-1.05510300	-0.07918900
C	0.28414100	2.50075900	-1.14498700
C	-1.10862300	2.36003300	-0.74853300
C	-1.47469100	2.58477200	0.55722300
C	-0.51894200	2.89277400	1.59185700
C	0.85018100	3.01226300	1.19676500
C	1.26240600	2.82349400	-0.12105300
C	-2.12823400	1.89152400	-1.78365100
C	2.73973700	2.79616500	-0.48055900
C	3.31409200	-2.13941800	0.98723700
C	-1.64738300	-2.79940000	0.00974200
O	-0.70907600	-0.64759000	-1.73362800
O	0.62713700	2.31122300	-2.37303500
O	1.09864600	-3.28609600	-0.55479900
O	3.11736900	0.74941900	1.49628800

O	1.85910500	-0.88234600	-3.29028900
O	0.09111800	0.07975800	3.65806400
O	-6.01979600	-0.56182500	-0.06516400
O	-0.89719100	3.01176800	2.82849100
H	-4.70940000	1.47502200	-1.12085100
H	-4.28557700	-2.48769500	0.44497000
H	-1.81561400	-1.15212800	2.19646200
H	2.34726600	-1.12128700	3.25311100
H	2.73923100	1.61091400	-2.91327700
H	3.19255300	-2.47697500	-1.67048600
H	-2.51344900	2.47280700	0.86356100
H	1.57869400	3.29589600	1.95734700
H	-1.63689100	1.82873300	-2.76026800
H	-2.91633000	2.64858700	-1.88469700
H	3.33465600	3.16104400	0.36173400
H	2.95183600	3.41858800	-1.35694500
H	3.96892400	-1.89058600	1.82803400
H	3.65969400	-3.07994200	0.54514200
H	-2.28325200	-3.51936300	0.54309500
H	-1.19809100	-3.35532500	-0.82056500
Li	-1.00547200	1.49669700	3.83064600
Li	0.55935600	-1.99432500	-1.87126700
Li	1.60581400	0.87476100	2.65477700
Li	0.33120600	0.45938100	-2.82639000
Li	1.69037600	-4.91766000	-0.84143400
Li	-7.65467100	-0.54646100	0.34404500

$C4QLi_7$ (by condensed Fukui function)

E= -1731.820349 hartrees

Symbol	X	Y	Z
C	-4.09251100	0.04082400	-1.12069900
C	-2.74026200	0.05727100	-1.50682100
C	-1.87322400	-1.02017500	-1.15654300
C	-2.38772000	-1.96467800	-0.22163900
C	-3.74193600	-1.94866500	0.15273300
C	-4.65671200	-0.98140100	-0.32315500
C	0.22764300	-0.40509100	2.88189700
C	-0.74494900	-1.16085100	2.18732800
C	-0.38366200	-2.20489600	1.32389600
C	0.99112000	-2.50625600	1.10463800
C	1.96869900	-1.81154700	1.86482100
C	1.55733000	-0.85935900	2.80826200

C	3.21241000	0.53329300	0.25179800
C	3.01625400	1.25140400	-1.00068200
C	2.94484500	0.55468900	-2.18796500
C	2.83337900	-0.87354800	-2.17092400
C	3.34906200	-1.55982000	-1.02554200
C	3.45658800	-0.91007000	0.18785500
C	0.14378400	2.18247000	-1.65157200
C	-1.22871500	2.06772700	-1.25340600
C	-1.65405000	2.55158400	-0.01236100
C	-0.76505500	3.13788000	0.91141000
C	0.59411600	3.20700500	0.54674000
C	1.06164300	2.73630200	-0.69761600
C	-2.19679500	1.31617000	-2.16706500
C	2.56325000	2.70337700	-0.98281800
C	3.43805300	-1.76873800	1.44708400
C	-1.44606400	-2.92126200	0.48721600
O	-0.61499800	-1.11723600	-1.63294400
O	0.53697300	1.74423100	-2.82968200
O	1.33908100	-3.34736700	0.10435700
O	3.12215400	1.15277500	1.37634900
O	2.06676100	-1.48954900	-3.02324600
O	-0.01188200	0.79772000	3.43660500
O	-5.94224200	-1.00024800	0.00126700
O	-1.20178300	3.56949900	2.13266000
H	-4.73499000	0.86958500	-1.42080700
H	-4.10348500	-2.69570700	0.86057700
H	-1.78688300	-0.84905900	2.24419800
H	2.31893600	-0.32193600	3.37085700
H	2.70350500	1.07879300	-3.10473600
H	3.41023100	-2.64240300	-1.06653900
H	-2.69966600	2.44789200	0.27782900
H	1.29827800	3.67514000	1.23922100
H	-1.67556900	1.09765900	-3.10535200
H	-3.04652100	1.96281200	-2.42585800
H	3.09449300	3.27655100	-0.21598300
H	2.77931400	3.15246800	-1.96033900
H	4.03759000	-1.33239000	2.25254200
H	3.84211900	-2.76017300	1.21426500
H	-2.04184300	-3.57654300	1.13838600
H	-0.93543500	-3.58458300	-0.21944600
Li	-1.21221100	2.11143500	3.24111400
Li	0.79375000	-2.32472000	-1.45440800
Li	1.44791800	1.44509200	2.22491200
Li	0.42248500	-0.11747900	-2.82756400

Li	2.01887500	-4.96070500	0.11653200
Li	-7.58604400	-1.02306400	0.35920400
Li	-1.71534700	5.22326500	2.45255100

$C4QLi_8$ (by condensed Fukui function)

E= -1739.420038 hartrees

Symbol	X	Y	Z
C	-4.18725500	0.12994200	-0.98771400
C	-2.84764900	0.08627200	-1.41662700
C	-2.00188000	-1.00576000	-1.05011500
C	-2.52140000	-1.89318300	-0.06044800
C	-3.86210700	-1.81645400	0.35393000
C	-4.75979000	-0.83899500	-0.13273900
C	0.27481200	-0.29647900	2.85036200
C	-0.75433500	-1.04076500	2.23278200
C	-0.47006200	-2.14918500	1.41847000
C	0.87770700	-2.53070200	1.16742400
C	1.91512300	-1.83461400	1.84661600
C	1.57921700	-0.81682000	2.75112100
C	3.25408600	0.39218000	0.08780500
C	2.98362400	1.03721600	-1.15103100
C	2.77859500	0.27715600	-2.31140400
C	2.61556600	-1.12516300	-2.24423100
C	3.14263900	-1.74904900	-1.09412500
C	3.38617300	-1.02690800	0.08934300
C	0.09021600	2.09298100	-1.77984300
C	-1.26496700	2.05786800	-1.31528100
C	-1.61731800	2.61617800	-0.08037700
C	-0.66590200	3.20504600	0.77398400
C	0.67950400	3.18509400	0.35236400
C	1.07643300	2.63230800	-0.88349500
C	-2.29339600	1.29813400	-2.15216700
C	2.56674200	2.50630800	-1.21128200
C	3.36892200	-1.85726800	1.37535200
C	-1.59072500	-2.85559600	0.65329700
O	-0.76851800	-1.16933500	-1.55943500
O	0.39954600	1.59734900	-2.95949900
O	1.14016400	-3.44812000	0.20979500
O	3.28255500	1.12106100	1.24212000
O	2.27373750	-1.83551315	-3.32356168
O	0.11634500	0.94559400	3.34617600
O	-6.03644800	-0.80182200	0.22986000

O	-1.02738300	3.72244300	1.98960900
H	-4.81248600	0.96627400	-1.30394400
H	-4.22550200	-2.52343300	1.10132200
H	-1.77816800	-0.67527300	2.30119500
H	2.38436100	-0.27930800	3.24865200
H	2.46917200	0.79316300	-3.21303400
H	3.12379600	-2.83358100	-1.04287400
H	-2.65329500	2.57095900	0.25707600
H	1.43325700	3.64438300	0.99732000
H	-1.80979800	1.01982800	-3.09449900
H	-3.13443800	1.95740200	-2.40962900
H	3.14291400	3.11450600	-0.50486400
H	2.76264900	2.88723500	-2.22241100
H	4.01140400	-1.43381700	2.15567600
H	3.72431700	-2.87155000	1.15839100
H	-2.18619100	-3.46365100	1.34996300
H	-1.12711500	-3.56013200	-0.04526000
Li	-1.00951300	2.31224900	3.15239500
Li	0.67596300	-2.39055800	-1.42202800
Li	1.54235700	1.39697700	1.94483900
Li	0.33966200	-0.28983700	-2.81658900
Li	1.80370100	-5.05476600	0.18680700
Li	-7.67228300	-0.77506000	0.61556400
Li	-1.47792600	5.40224900	2.24066800
Li	1.58398459	-2.66555321	-4.52519361

$C4QLi_1$ (by lowest energy method)

E= -1686.127449 hartrees

Symbol	X	Y	Z
C	-4.21389000	1.27002400	-1.13089400
C	-2.86589200	1.29431300	-1.14450100
C	-2.11475500	-0.00027800	-1.24683300
C	-2.86593800	-1.29476200	-1.14399700
C	-4.21394700	-1.27035300	-1.13043400
C	-4.97734400	-0.00015900	-1.16141300
C	-0.41029400	-1.97125100	2.39031100
C	-1.39685300	-2.17973300	1.34684000
C	-1.03757300	-2.50383400	0.07465300
C	0.38804000	-2.76850000	-0.24609600
C	1.39492800	-2.50093800	0.81000100
C	0.99049700	-2.15798900	2.06393300
C	3.23361500	-0.00002500	0.38774000

C	3.19091800	1.28622200	-0.37610900
C	3.41160200	1.26756500	-1.70558100
C	3.62600700	-0.00059400	-2.44252900
C	3.41161800	-1.26843700	-1.70507300
C	3.19089600	-1.28658000	-0.37559600
C	0.38820300	2.76843200	-0.24714200
C	-1.03745700	2.50382000	0.07369900
C	-1.39667500	2.18036900	1.34604300
C	-0.41009000	1.97251000	2.38969400
C	0.99068500	2.15891300	2.06323300
C	1.39510700	2.50124600	0.80914200
C	-2.03456100	2.55360800	-1.06873200
C	2.85531600	2.54194000	0.40619600
C	2.85518100	-2.54193700	0.40718300
C	-2.03482500	-2.55417300	-1.06762900
O	-0.89871600	-0.00032600	-1.40187400
O	0.72508600	3.20178900	-1.35756300
O	0.72488100	-3.20223900	-1.35645600
O	3.30071600	0.00020400	1.61633600
O	3.92865600	-0.00081900	-3.63382500
O	-0.76296000	-1.56450300	3.54186400
O	-6.20638100	-0.00013500	-1.16991700
O	-0.76281200	1.56627700	3.54142600
H	-4.81065300	2.17805100	-1.08239000
H	-4.81075700	-2.17833200	-1.08159400
H	-2.43435800	-1.99092000	1.61492100
H	1.71225200	-1.94771800	2.84812400
H	3.41291700	2.17467200	-2.30370700
H	3.41293900	-2.17578900	-2.30282700
H	-2.43414100	1.99162200	1.61433500
H	1.71250700	1.94894500	2.84744400
H	-1.46773800	2.69088000	-1.99639000
H	-2.70231200	3.41764800	-0.96428400
H	3.47923100	2.60017000	1.30327000
H	3.04648200	3.41627200	-0.22214700
H	3.47898500	-2.59985800	1.30435000
H	3.04633300	-3.41656300	-0.22076800
H	-2.70276900	-3.41797200	-0.96245900
H	-1.46819200	-2.69216800	-1.99529500
Li	-0.91119900	0.00085400	4.36760600

$C4QLi_2$ (by lowest energy method)

E= -1693.711664 hartrees

Symbol	X	Y	Z
C	-4.06721600	1.41846800	-0.58636200
C	-2.75370900	1.39466600	-0.90338800
C	-2.15265000	0.10158700	-1.35355200
C	-2.88188800	-1.16570100	-1.05067500
C	-4.19187300	-1.09477600	-0.72090600
C	-4.89467000	0.19289300	-0.55675300
C	-0.19465600	-2.19200800	2.28940600
C	-1.24720000	-2.28942800	1.31383800
C	-0.98202200	-2.41866800	-0.02899900
C	0.39398400	-2.47305800	-0.50683900
C	1.45851500	-2.52172900	0.48629800
C	1.15025300	-2.36550700	1.82309500
C	3.34523100	-0.05278500	0.21137200
C	3.16521300	1.28461200	-0.44104500
C	2.90643300	1.36535500	-1.77256900
C	2.65819600	0.14890900	-2.54381200
C	3.04760400	-1.13239700	-1.97507400
C	3.19404100	-1.26735700	-0.63223200
C	0.55905300	2.81574900	0.02499700
C	-0.83987400	2.41788000	0.32442900
C	-1.14070200	1.90209900	1.54716900
C	-0.11348100	1.63634700	2.54681700
C	1.27066200	1.89753200	2.19827300
C	1.61617500	2.42272900	0.98905900
C	-1.85329800	2.59683800	-0.79655900
C	3.04467300	2.47992400	0.48510200
C	2.91659700	-2.58876700	0.04085000
C	-2.09890200	-2.45281300	-1.06593800
O	-1.08393800	0.09465700	-1.98508300
O	0.82959400	3.43914900	-1.01032500
O	0.63471200	-2.44550400	-1.76756200
O	3.60649700	-0.13838600	1.41497400
O	1.92745600	0.16412200	-3.57040600
O	-0.45654100	-1.94266900	3.52632700
O	-6.10551900	0.24394200	-0.33950200
O	-0.42568600	1.13357300	3.66682600
H	-4.57353700	2.34116400	-0.31251100
H	-4.78478400	-1.98821000	-0.53995200
H	-2.26999100	-2.21887000	1.67946300
H	1.94269000	-2.33431400	2.56599000
H	2.67815400	2.31293400	-2.25060500
H	2.92742600	-2.00175800	-2.61171900

H	-2.15615400	1.62028700	1.81573700
H	2.02739800	1.59521800	2.91628800
H	-1.29749800	2.75994500	-1.72462100
H	-2.46135100	3.49403000	-0.62599700
H	3.74663800	2.39973200	1.31825600

$C4QLi_3$ (by lowest energy method)

E= -1701.35297 hartrees

Symbol	X	Y	Z
C	-4.09705200	1.22520300	-0.64297500
C	-2.77212400	1.23678700	-1.01504300
C	-2.10391100	-0.00134600	-1.34409600
C	-2.77246800	-1.23875500	-1.01283000
C	-4.09737900	-1.22619300	-0.64085100
C	-4.85733100	-0.00025500	-0.49648600
C	-0.20613600	-2.07378100	2.43857200
C	-1.22444200	-2.25065900	1.43432400
C	-0.91358800	-2.50327800	0.12362000
C	0.48053600	-2.65419000	-0.27280000
C	1.51669700	-2.55407900	0.74878000
C	1.16499400	-2.28722400	2.05011900
C	3.35225500	-0.00008200	0.29823400
C	3.20811000	1.29170700	-0.45819000
C	3.04051200	1.25635000	-1.80248700
C	2.62480200	-0.00343000	-2.40170100
C	3.04042200	-1.26172600	-1.79934200
C	3.20780500	-1.29370300	-0.45494900
C	0.48119000	2.65370600	-0.27849900
C	-0.91286000	2.50346100	0.11870600
C	-1.22331000	2.25387000	1.43006000
C	-0.20470700	2.07986100	2.43455500
C	1.16631400	2.29204500	2.04504700
C	1.51766400	2.55561500	0.74292000
C	-1.98988700	2.53748800	-0.96063700
C	2.98577300	2.56918100	0.31841300
C	2.98490700	-2.56915800	0.32476900
C	-1.99042400	-2.53947600	-0.95584700
O	-0.90184400	-0.00206700	-1.90248200
O	0.78398500	2.80537100	-1.51634800
O	0.78380300	-2.80831700	-1.51029500
O	3.61408600	0.00138600	1.49653900
O	1.69759700	-0.00457900	-3.26366200

O	-0.50118100	-1.66556100	3.61879400
O	-6.07916100	0.00016600	-0.19463100
O	-0.49942200	1.67547400	3.61621100
H	-4.61803900	2.15214800	-0.41409800
H	-4.61861600	-2.15258400	-0.41030200
H	-2.25589300	-2.09430800	1.74181100
H	1.92496000	-2.14788300	2.81441600
H	2.89231800	2.16377400	-2.37528700
H	2.89241800	-2.17064100	-2.36983100
H	-2.25468200	2.09830200	1.73822200
H	1.92651200	2.15453600	2.80944500
H	-1.52888800	2.79109800	-1.92113600
H	-2.69165000	3.35172600	-0.74568900
H	3.62314400	2.61117200	1.20520600
H	3.20069200	3.43115300	-0.32127200
H	3.62206400	-2.60914100	1.21180900
H	3.19966000	-3.43276000	-0.31276100
H	-2.69233600	-3.35316400	-0.73932400
H	-1.52935900	-2.79509100	-1.91578600
Li	-0.69203900	0.00544500	4.22260100
Li	0.22694800	-1.35158800	-2.53911000
Li	0.22729800	1.34582100	-2.54240800

$C4QLi_4$ (by lowest energy method)

E= -1708.926161 hartrees

Symbol	X	Y	Z
C	-4.26284800	0.37936000	-0.86053200
C	-2.96230400	0.41035300	-1.26082300
C	-2.12293700	-0.79172000	-1.04752300
C	-2.60695900	-1.81105300	-0.08825300
C	-3.91178500	-1.80536100	0.28434700
C	-4.84970000	-0.75669100	-0.14313100
C	0.39996600	-0.57262100	2.87263300
C	-0.69577600	-1.19963500	2.19959300
C	-0.48088700	-2.16999100	1.23970600
C	0.86527100	-2.53607200	0.84665900
C	1.95376600	-1.99656300	1.62030600
C	1.68392400	-1.11354000	2.66497800
C	3.13263000	0.29544900	0.07311400
C	2.89246600	1.11514200	-1.12027100
C	2.67267800	0.49973900	-2.32516400
C	2.44147600	-0.92059400	-2.36079200

C	3.03846300	-1.72045400	-1.33406900
C	3.30699500	-1.15839500	-0.10454300
C	0.07390900	2.20958700	-1.37975800
C	-1.28783400	2.21585000	-0.88337300
C	-1.57120400	2.66178500	0.39052900
C	-0.53953700	3.07145900	1.29682800
C	0.80007800	3.09174300	0.78430100
C	1.12408400	2.68061900	-0.50563400
C	-2.36472000	1.67903400	-1.81839800
C	2.57377700	2.58955700	-0.96663600
C	3.37879400	-2.07713900	1.10100900
C	-1.63387000	-2.81287600	0.48183000
O	-1.02820300	-0.97438600	-1.67090800
O	0.31804400	1.76511400	-2.56742400
O	1.05905100	-3.26065200	-0.21212300
O	3.16430200	0.83706100	1.22190400
O	1.53824900	-1.41266400	-3.15540100
O	0.28023800	0.57797400	3.52688600
O	-6.05073700	-0.80005400	0.14908200
O	-0.80173600	3.36431100	2.53606600
H	-4.92363600	1.22340400	-1.04119400
H	-4.31160000	-2.56690700	0.94957400
H	-1.70316600	-0.84705200	2.41421600
H	2.51127500	-0.70526300	3.24120900
H	2.44122400	1.08196800	-3.20832100
H	3.05653500	-2.79661700	-1.45980200
H	-2.59424200	2.67320000	0.76255200
H	1.57759500	3.50019900	1.43360900
H	-1.92339900	1.53011800	-2.80815700
H	-3.16860700	2.41399200	-1.93741600
H	3.22733100	3.07093600	-0.23357300
H	2.70294200	3.09181200	-1.93179500
H	4.08418600	-1.72558400	1.85922900
H	3.66070700	-3.08597300	0.78640900
H	-2.18900500	-3.48154600	1.15160400
H	-1.21182100	-3.45282600	-0.30013500
Li	-0.77105200	2.01695700	3.68916000
Li	0.50917600	-2.40901900	-1.76307200
Li	0.12871000	-0.01303800	-2.97403400
Li	1.68066700	1.25865800	2.29986300

$C4QLi_5$ (by lowest energy method)

E= -1716.558307 hartrees

Symbol	X	Y	Z
C	-4.07660400	0.69693100	-0.89132200
C	-2.74732800	0.70880800	-1.31404800
C	-1.96526400	-0.48892800	-1.29978800
C	-2.54380800	-1.61871600	-0.64152000
C	-3.87534500	-1.59371800	-0.21819200
C	-4.69986200	-0.46278800	-0.38121600
C	0.22902300	-1.30031900	2.70581700
C	-0.83600100	-1.72710600	1.86466300
C	-0.58480000	-2.44392800	0.70937900
C	0.79011600	-2.73136100	0.31780000
C	1.85765300	-2.40726400	1.24916600
C	1.53398100	-1.80929400	2.44862800
C	3.23973700	0.20665500	0.29059600
C	3.10937500	1.26343500	-0.70170200
C	2.95506700	0.94074500	-2.03136700
C	2.69614700	-0.41786000	-2.40039400
C	3.17783700	-1.44280100	-1.52181400
C	3.36544600	-1.17215500	-0.18673200
C	0.31555600	2.54331700	-0.93619300
C	-1.08208400	2.41302000	-0.54904200
C	-1.44018400	2.52267700	0.77116200
C	-0.46812700	2.70644900	1.81259800
C	0.90827000	2.84899000	1.42182800
C	1.31842200	2.74468100	0.10753000
C	-2.10020500	2.04693800	-1.62261000
C	2.79775600	2.68488300	-0.25520100
C	3.30520300	-2.34953300	0.78161600
C	-1.69105100	-2.81378900	-0.26886600
O	-0.73568600	-0.53176500	-1.83057500
O	0.64946300	2.42998700	-2.16518800
O	1.04208500	-3.15981100	-0.86400100
O	3.18208600	0.48161700	1.54630600
O	1.82877200	-0.69982200	-3.32682000
O	0.11985600	-0.30855100	3.57735500
O	-5.97816600	-0.47005500	-0.03159800
O	-0.80281900	2.65073900	3.06216700
H	-4.66079300	1.61511500	-0.93125500
H	-4.30203800	-2.47419200	0.25994900
H	-1.84562000	-1.38276300	2.08040500
H	2.32879500	-1.53438900	3.14018700
H	2.76476800	1.71658600	-2.76282600
H	3.13451100	-2.46991900	-1.86724700

H	-2.47612000	2.38949300	1.07534800
H	1.63759900	3.03936800	2.21068500
H	-1.60730300	2.06372200	-2.59913900
H	-2.88119300	2.81625600	-1.66047100
H	3.39791100	2.97256700	0.61291100
H	3.01554300	3.37647200	-1.07630800
H	3.96442100	-2.20432700	1.64297900
H	3.60279800	-3.26310000	0.25801800
H	-2.33472800	-3.57657800	0.18827400
H	-1.23344900	-3.29126500	-1.14107800
Li	-0.95298900	1.08930200	3.89365500
Li	0.52248300	-1.87456000	-2.19636500
Li	0.37027400	0.63488400	-2.79244600
Li	1.67246000	0.58281300	2.58018600
Li	-7.57336100	-0.50563800	0.26955000

$C4QLi_6$ (by lowest energy method)

E= -1724.172598 hartrees

Symbol	X	Y	Z
C	-4.12282700	0.65920000	-0.89035300
C	-2.78108900	0.70304000	-1.28124800
C	-1.97693600	-0.47056300	-1.25917600
C	-2.53841200	-1.61316800	-0.62713500
C	-3.88257500	-1.62787600	-0.23437700
C	-4.72817300	-0.51529000	-0.40090400
C	0.27423500	-1.26723600	2.70581900
C	-0.77661800	-1.69509500	1.85173000
C	-0.52937200	-2.42214700	0.69143300
C	0.81658500	-2.69575000	0.31397700
C	1.87289500	-2.36910500	1.21022800
C	1.56062300	-1.75555600	2.43850800
C	3.14857100	0.35978500	0.26406000
C	3.01968400	1.41656200	-0.72194500
C	2.84423800	1.10160900	-2.06065000
C	2.59879000	-0.25101000	-2.44194400
C	3.11536900	-1.27538600	-1.56907500
C	3.30376700	-1.01741500	-0.23640200
C	0.26943600	2.60354900	-0.91245800
C	-1.12120800	2.41869600	-0.51392500
C	-1.46926000	2.50362100	0.80707300
C	-0.49413900	2.70719000	1.85267100
C	0.87262600	2.87719800	1.45711800

C	1.26909500	2.82417300	0.12792900
C	-2.14736500	2.04943800	-1.57806100
C	2.73656100	2.83376800	-0.25974000
C	3.32458700	-2.19409300	0.72345500
C	-1.65766000	-2.79245200	-0.26791400
O	-0.72429100	-0.47860100	-1.75954400
O	0.59436900	2.53379200	-2.14739600
O	1.10156600	-3.23509800	-0.90383800
O	3.11065000	0.60440100	1.52153700
O	1.77049800	-0.57197800	-3.38485400
O	0.13198700	-0.28932900	3.61303400
O	-6.01492700	-0.55114000	-0.06159700
O	-0.84498100	2.67071500	3.09689700
H	-4.72405300	1.56657400	-0.93439500
H	-4.29551000	-2.52251900	0.23046100
H	-1.79131100	-1.36175300	2.06105600
H	2.37150900	-1.47870700	3.10956300
H	2.67559400	1.88365500	-2.78931700
H	3.12999000	-2.29198100	-1.94851300
H	-2.49970400	2.34402300	1.11740600
H	1.60231700	3.09787300	2.23674900
H	-1.66655000	2.08293400	-2.56103600
H	-2.93430700	2.81392200	-1.59972700
H	3.35054000	3.11576200	0.60054000
H	2.92677000	3.53585000	-1.07853100
H	3.97059700	-2.01554300	1.58763000
H	3.75510900	-3.05950100	0.18541900
H	-2.28377100	-3.56462500	0.19989200
H	-1.21791900	-3.26171400	-1.15493600
Li	-0.93423500	1.09106100	3.91614700
Li	0.54581300	-1.79452200	-2.09943600
Li	0.31053600	0.71482200	-2.76082700
Li	1.58163400	0.61009700	2.59145800
Li	-7.60156300	-0.56624700	0.24503700
Li	2.03886700	-4.36203300	0.04483600

$C4QLi_7$ (by lowest energy method)

E= -1731.805782 hartrees

Symbol	X	Y	Z
C	-4.05541300	0.54967800	-1.36154000
C	-2.66981900	0.68583700	-1.52184000
C	-1.80913700	-0.44260700	-1.40154200

C	-2.41054600	-1.65282200	-0.95597200
C	-3.79975800	-1.75104000	-0.79641100
C	-4.66711400	-0.67163100	-1.03214500
C	-0.10848100	-1.45237500	2.73690200
C	-1.02481900	-1.86637700	1.73913000
C	-0.61062500	-2.55517500	0.59781800
C	0.77206900	-2.81226600	0.40988200
C	1.70427200	-2.43150900	1.41285200
C	1.22544300	-1.87830100	2.61145500
C	2.89948000	0.38923900	0.67856300
C	2.83785500	1.48436500	-0.24108300
C	3.05710300	1.28514700	-1.61257100
C	3.32452800	0.01216700	-2.16362900
C	3.37163400	-1.07159100	-1.25947700
C	3.18255000	-0.90438600	0.12264900
C	0.09037400	2.81415500	-0.64865500
C	-1.31813700	2.51627000	-0.46425400
C	-1.84312300	2.47895600	0.80488300
C	-1.02278400	2.64253700	1.97388100
C	0.38445600	2.87795200	1.77687300
C	0.95058800	2.91074000	0.52105500
C	-2.12227000	2.09488800	-1.68682000
C	2.45006000	2.86361700	0.28731800
C	3.16637200	-2.12393400	1.03818800
C	-1.56917400	-2.84965800	-0.55202800
O	-0.47214100	-0.36379000	-1.65508300
O	0.59096600	2.87639000	-1.83136300
O	1.24247000	-3.31790800	-0.77277100
O	2.68927300	0.56614600	1.96072200
O	3.53383500	-0.15436800	-3.47375300
O	-0.39885800	-0.51254700	3.65254200
O	-5.98987800	-0.78656700	-0.90707000
O	-1.50772400	2.46086800	3.16111500
H	-4.69132100	1.42707200	-1.47354100
H	-4.23206500	-2.69460900	-0.46515200
H	-2.06079200	-1.54080600	1.81160000
H	1.94309300	-1.56976200	3.36847100
H	3.04108000	2.14224700	-2.28240400
H	3.60718900	-2.05767000	-1.65813900
H	-2.88706100	2.21709800	0.96315100
H	1.00847300	2.98337900	2.66456600
H	-1.48750000	2.19855800	-2.57289200
H	-2.96450000	2.78248800	-1.83366000
H	2.97188800	3.05864600	1.22974200

H	2.73969300	3.62737200	-0.44284700
H	3.72507800	-1.92151600	1.95766500
H	3.71265800	-2.94023100	0.52262600
H	-2.24569500	-3.66492200	-0.26172900
H	-0.98457500	-3.23951500	-1.39347400
Li	-1.54761400	0.81613900	3.85733500
Li	0.85603400	-1.63609800	-1.51318900
Li	0.64680800	1.02439800	-2.05259400
Li	1.14304000	0.47364700	2.84741900
Li	-7.59540500	-0.88611600	-0.79835100
Li	2.22974100	-4.30103000	0.27431700
Li	3.92982800	-0.09256500	-5.04480400

$C4QLi_8$ (by lowest energy method)

E= -1731.805782 hartrees

Symbol	X	Y	Z
C	-4.01009400	0.08124000	-1.49719900
C	-2.62771600	0.25395200	-1.66405900
C	-1.72086800	-0.80122500	-1.34981200
C	-2.28085700	-1.94633800	-0.71414300
C	-3.66722300	-2.07989200	-0.55571700
C	-4.57517700	-1.09614500	-0.98010200
C	-0.05228000	-1.00913100	2.89920700
C	-0.93185900	-1.63171000	1.98134200
C	-0.46843500	-2.48853500	0.98130400
C	0.92693300	-2.70872200	0.85272400
C	1.82423100	-2.12531600	1.78972900
C	1.30016400	-1.39132100	2.86729600
C	2.93212800	0.57282100	0.63370600
C	2.80978100	1.50280000	-0.44787800
C	3.06374800	1.10214900	-1.76631900
C	3.40788900	-0.22651200	-2.10705600
C	3.49388500	-1.15112400	-1.04658600
C	3.27793900	-0.77445100	0.29303100
C	-0.00056500	2.62519900	-1.11972100
C	-1.37407200	2.29820500	-0.91411100
C	-1.93678500	2.40317000	0.36744100
C	-1.17061700	2.78624500	1.49157200
C	0.20518400	3.03522200	1.30302400
C	0.80173100	2.90432500	0.04178900
C	-2.13768800	1.63856100	-2.05501600
C	2.31240700	2.91449600	-0.14443800

C	3.28477700	-1.82894000	1.39358600
C	-1.39362200	-3.01823800	-0.10922700
O	-0.38905600	-0.71071700	-1.59828500
O	0.54343300	2.52501300	-2.30603100
O	1.43834300	-3.37729100	-0.22620500
O	2.70708900	0.94188800	1.87489100
O	3.63956700	-0.58264300	-3.37722400
O	-0.40187300	0.06734900	3.62795100
O	-5.89762800	-1.25680200	-0.86536700
O	-1.81156200	2.95284500	2.71183100
H	-4.68232300	0.89430100	-1.77204400
H	-4.06437400	-2.97585000	-0.07906200
H	-1.98180600	-1.34485200	1.98505100
H	1.98897300	-0.91882700	3.56281100
H	2.99294400	1.83801000	-2.56380400
H	3.78043500	-2.17569000	-1.28266100
H	-2.94524400	2.00538600	0.52998100
H	0.81023400	3.34002700	2.15932300
H	-1.47946100	1.62379200	-2.93003100
H	-3.00664100	2.24723600	-2.34196700
H	2.79635900	3.28362300	0.76629400
H	2.57240200	3.57486400	-0.97952500
H	3.81401500	-1.45961800	2.27799000
H	3.87332700	-2.69704200	1.02852100
H	-2.03684400	-3.80520500	0.30831500
H	-0.77663900	-3.51115500	-0.86909000
Li	-1.57297400	1.37500200	3.56277800
Li	1.03322700	-1.83051200	-1.23249100
Li	0.65210100	0.70897500	-2.17082600
Li	1.07909600	0.96036100	2.59618400
Li	-7.47435000	-1.58217200	-0.84115000
Li	2.47256300	-4.10969100	0.96867100
Li	3.95474300	-0.65197100	-4.96337700
Li	-2.82424000	3.98305500	1.72061200

P5Q

E= -2098.040382 hartrees

Symbol	X	Y	Z
C	3.90549900	-1.52513300	1.24124900
C	4.19270900	-0.07338700	1.21516300
C	4.33496200	0.61353700	0.06562100
C	4.19253500	-0.10689800	-1.24147400

C	3.89408800	-1.55638000	-1.21539000
C	3.75826800	-2.24460000	-0.06584400
C	4.59516900	2.10391800	-0.00019900
C	3.42051300	-3.71934400	0.00008100
C	3.29652300	2.88014100	-0.06578000
C	2.68364000	3.22187100	-1.21519300
C	1.39667100	3.95248400	-1.24098900
C	0.75592400	4.31080300	0.06623100
C	1.36546000	3.96314900	1.21564300
C	2.65743000	3.24140300	1.24145400
C	-0.58093600	5.01915500	0.00055100
C	-1.72095700	4.02454500	-0.06556700
C	-2.26349700	3.52934400	1.24142300
C	-3.34911400	2.52360300	1.21516200
C	-3.86751000	2.05123000	0.06551900
C	-3.32814900	2.54989300	-1.24147500
C	-2.23485500	3.54728200	-1.21520500
C	-4.95430300	0.99872000	-0.00057700
C	-4.06505700	-1.02930100	-1.21564100
C	-3.45408300	-2.37719600	-1.24142900
C	-3.14624000	-3.04367400	0.06579100
C	-3.43556600	-2.40438400	1.21520900
C	-4.05710500	-1.06132700	1.24100200
C	-4.36036000	-0.39274600	-0.06623200
C	-2.48069300	-4.40235500	0.00017400
C	1.19336800	-4.01840300	-1.24121200
C	1.92259300	-3.93193200	0.06590200
C	1.22533400	-4.00932200	1.21541700
C	-0.24408800	-4.18505000	1.24144400
C	-0.97380700	-4.26722600	-0.06566500
C	-0.27733200	-4.18309100	-1.21518500
O	1.79848700	-3.95079000	-2.30661700
O	3.78894600	-2.12271500	2.30667500
O	0.86773900	4.25442500	-2.30630000
O	-1.81727500	3.94336900	2.30692600
O	-3.20264200	-2.93191200	-2.30674200
O	4.31684600	0.48912300	-2.30689900
O	3.18986200	2.94569400	2.30676800
O	-3.77838500	2.14025600	-2.30698600
O	-4.31271700	-0.50853300	2.30632100
O	-0.84851900	-4.25848600	2.30685100
H	4.26746900	0.41042400	2.18503100
H	3.77598600	-2.03145100	-2.18526800
H	5.18977600	2.31898700	-0.89111100

H	5.14640900	2.41383500	0.89065300
H	3.88542100	-4.14787800	0.89100300
H	3.80854900	-4.21874400	-0.89073900
H	3.09912100	2.96337400	-2.18516900
H	0.92865000	4.18376800	2.18560500
H	-0.60133900	5.65135800	-0.89019600
H	-0.70523800	5.63900900	0.89154200
H	-3.69445900	2.17649800	2.18499200
H	-1.85969700	3.86194200	-2.18502900
H	-5.56152000	1.17451500	-0.89159400
H	-5.58258500	1.07206900	0.89015800
H	-3.21207300	-2.83969300	2.18519200
H	-4.24845000	-0.57562900	-2.18562200
H	-2.83545400	-4.92592800	-0.89063900
H	-2.74444500	-4.97698400	0.89111100
H	1.70857100	-3.93142500	2.18532600
H	-0.76561800	-4.21747200	-2.18508600

P5QLi$_1$ (by condensed Fukui function)

E= -2105.659569 hartrees

Symbol	X	Y	Z
C	2.25355000	3.76367400	-1.06310200
C	3.41917600	2.88609800	-1.14475300
C	3.85221000	2.11066200	-0.10797700
C	3.05917200	2.09094000	1.13237600
C	1.93829600	3.00963600	1.25022000
C	1.54692700	3.82881100	0.24019000
C	5.09408400	1.24135300	-0.26797600
C	0.38960100	4.79859200	0.35145800
C	4.65924900	-0.19793600	-0.24674700
C	4.65064000	-0.90073100	0.91865800
C	3.76833900	-2.02401700	1.11380200
C	3.29410900	-2.74521400	-0.07455800
C	3.44115600	-2.14419200	-1.28561200
C	4.04739300	-0.80607400	-1.44966100
C	2.61350700	-4.08877300	0.12745500
C	1.10373900	-4.00030500	0.14529800
C	0.39724900	-4.09153700	-1.17463400
C	-1.08092600	-4.01516200	-1.18810600
C	-1.80847000	-3.89134100	-0.06182300
C	-1.10389900	-3.79784300	1.25769500
C	0.37423200	-3.85699400	1.26852800

C	-3.32037700	-3.80175100	-0.04277400
C	-4.06656300	-1.67520200	1.09108900
C	-4.46095900	-0.24986200	1.07078600
C	-4.49840200	0.45888700	-0.24994500
C	-4.22510400	-0.22963300	-1.37484300
C	-3.87480100	-1.66749000	-1.35872300
C	-3.77925900	-2.35957100	-0.03188600
C	-4.78604100	1.94423300	-0.21825200
C	-1.65869300	3.63406300	1.37062500
C	-0.93964600	4.10755100	0.14412200
C	-1.47509700	3.86344600	-1.06832400
C	-2.75862900	3.14981900	-1.23920100
C	-3.49734100	2.71272800	-0.00783500
C	-2.96397300	2.95900000	1.20371000
O	-1.17326300	3.78621200	2.48843100
O	1.88055600	4.44379200	-2.03130800
O	3.33251400	-2.26401600	2.28743800
O	1.02563000	-4.23535100	-2.21843400
O	-4.73764100	0.33762300	2.11231700
O	3.32042500	1.31465800	2.10668900
O	4.05823300	-0.22993700	-2.54373300
O	-1.73459300	-3.68017700	2.30464200
O	-3.65864000	-2.27498900	-2.40258400
O	-3.20995200	2.91760900	-2.35669000
H	3.94422000	2.88834700	-2.09508500
H	1.41638000	3.00966800	2.20409000
H	5.79930200	1.43012300	0.54982800
H	5.57871600	1.49323100	-1.21433900
H	0.51765300	5.56908600	-0.41233700
H	0.39315900	5.25869300	1.34278300
H	5.13893500	-0.49545300	1.80249800
H	3.06181000	-2.60955200	-2.19101300
H	2.95335100	-4.51787000	1.07349100
H	2.90966400	-4.75424700	-0.68829200
H	-1.54551200	-4.05961600	-2.16899600
H	0.84167900	-3.78512800	2.24702900
H	-3.69399400	-4.30587300	0.85192100
H	-3.72026300	-4.29496800	-0.93202200
H	-4.22824200	0.24471800	-2.35246000
H	-3.99979600	-2.13212700	2.07416000
H	-5.47602100	2.15620300	0.60203600
H	-5.23332100	2.25237500	-1.16561500
H	-0.97373900	4.16672200	-1.98383100
H	-3.45035200	2.63717400	2.12027400

Li	3.10450800	-0.39003700	2.72869100

P5QLi$_2$ (by condensed Fukui function)

E= -2113.337714 hartrees

Symbol	X	Y	Z
C	-3.22146400	-2.76135200	-1.00418200
C	-4.40481800	-1.97825100	-0.87183500
C	-4.63419600	-1.14603300	0.20576200
C	-3.71552200	-1.20088200	1.33589600
C	-2.71711400	-2.26260200	1.32067600
C	-2.48204900	-3.04785800	0.22642300
C	-5.59671500	0.00019900	-0.00106800
C	-1.50836200	-4.21327700	0.20991200
C	-4.63392400	1.14636000	-0.20705200
C	-4.40549100	1.97873500	0.87060200
C	-3.22221500	2.76181100	1.00395200
C	-2.48154100	3.04794300	-0.22598000
C	-2.71560200	2.26241800	-1.32029700
C	-3.71418100	1.20095500	-1.33629200
C	-1.50774800	4.21328100	-0.20856700
C	-0.04939400	3.84094300	-0.07370400
C	0.73574000	3.67832900	-1.33981200
C	2.18865500	3.41739600	-1.23757300
C	2.81523600	3.28232000	-0.05338700
C	2.01797500	3.37927800	1.21399800
C	0.57392600	3.67640500	1.10962400
C	4.28811200	2.95328100	0.08422700
C	4.48802000	0.71906100	1.23810300
C	4.52638900	-0.75873400	1.21958700
C	4.46077300	-1.45181400	-0.10896700
C	4.48752200	-0.71947200	-1.23840000
C	4.52619300	0.75831100	-1.21990200
C	4.46111000	1.45141000	0.10867900
C	4.28749300	-2.95364800	-0.08453300
C	0.73541300	-3.67824100	1.34047200
C	-0.05002300	-3.84097900	0.07454400
C	0.57298500	-3.67646100	-1.10894700
C	2.01699600	-3.37935000	-1.21368300
C	2.81460400	-3.28248400	0.05348200
C	2.18832700	-3.41743800	1.23784400
O	0.19168400	-3.75874400	2.43807000
O	-2.79141600	-3.09624600	-2.16777400

O	-2.79339300	3.09688200	2.16796800
O	0.19174800	3.75896200	-2.43727800
O	4.58367200	-1.40019400	2.26422000
O	-3.76598300	-0.38510300	2.32103000
O	-3.76400900	0.38497800	-2.32138800
O	2.55455600	3.22784500	2.30807400
O	4.58325500	1.39976300	-2.26455000
O	2.55330500	-3.22788900	-2.30789800
H	-5.06668200	-1.92693500	-1.73413400
H	-2.14275300	-2.40517800	2.23288600
H	-6.23401900	0.19629800	0.86613900
H	-6.23325300	-0.19582200	-0.86884900
H	-1.77503700	-4.86331400	-0.62760100
H	-1.62839900	-4.77348400	1.14174600
H	-5.06820100	1.92772800	1.73228100
H	-2.14033700	2.40473700	-2.23197400
H	-1.77434600	4.86250300	0.62959000
H	-1.62792700	4.77438000	-1.13986700
H	2.71755900	3.31603700	-2.18103100
H	0.03706400	3.76986400	2.05020700
H	4.66739900	3.38441800	1.01331100
H	4.83603100	3.36649900	-0.76584300
H	4.43923400	-1.17912000	-2.22143800
H	4.44010100	1.17870700	2.22115900
H	4.83560000	-3.36703300	0.76533700
H	4.66643100	-3.38478800	-1.01375800
H	0.03582100	-3.76988200	-2.04935600
H	2.71750500	-3.31608500	2.18114900
Li	-3.13486500	1.28438700	2.75400200
Li	-3.13173800	-1.28402600	-2.75445200

P5QLi$_3$ (by condensed Fukui function)

E= -2120.955661 hartrees

Symbol	X	Y	Z
C	1.88569700	-4.01686200	0.95308100
C	3.22749800	-3.50622000	0.94477200
C	3.67695400	-2.67003800	-0.04396000
C	2.83452100	-2.48192200	-1.21559900
C	1.69599300	-3.36081900	-1.36752100
C	1.20427300	-4.10766800	-0.32488700
C	4.85752800	-1.76528300	0.25109800
C	-0.08885000	-4.89952700	-0.40171900

C	4.40066900	-0.31946700	0.38991700
C	5.03555200	0.66153600	-0.39418700
C	4.57213200	1.98897800	-0.52700700
C	3.34956500	2.30514300	0.13625100
C	2.73492600	1.34476700	0.95135200
C	3.24714400	0.03168300	1.17810500
C	2.81199200	3.72585000	0.00852700
C	1.31142600	3.85072200	-0.05386400
C	0.56737900	4.06860600	1.23197100
C	-0.91151200	4.13979200	1.18971400
C	-1.60549800	4.08665500	0.03746900
C	-0.86339400	3.93812300	-1.25543900
C	0.60811100	3.81744200	-1.20391700
C	-3.11753900	4.12108800	-0.03898500
C	-3.96487400	2.04450300	-1.19632700
C	-4.45031900	0.64671000	-1.18713300
C	-4.56456100	-0.05647300	0.13193300
C	-4.28483300	0.61744500	1.26400400
C	-3.85746200	2.03355800	1.25847100
C	-3.67433300	2.71406800	-0.06514400
C	-4.95105200	-1.51846300	0.09490600
C	-2.02459100	-3.57345800	-1.45652200
C	-1.31907500	-4.03832100	-0.21829500
C	-1.79448900	-3.66138900	0.98631800
C	-2.99571900	-2.81793000	1.14049400
C	-3.72638000	-2.38975800	-0.09784200
C	-3.24567000	-2.74898600	-1.30271200
O	-1.60949200	-3.86482100	-2.57401900
O	1.28688200	-4.17650200	2.08057800
O	5.24127500	2.88702600	-1.24102100
O	1.16646600	4.19299700	2.29433800
O	-4.74205700	0.07830200	-2.23492100
O	3.03305100	-1.52830500	-2.05837000
O	2.65798100	-0.77833300	2.01309900
O	-1.45983800	3.91827700	-2.32922400
O	-3.65128500	2.63362800	2.30904800
O	-3.39315600	-2.47549900	2.25207600
H	3.78744400	-3.59474100	1.87562400
H	1.15736500	-3.30846200	-2.31067500
H	5.60680800	-1.81889200	-0.54773900
H	5.33781500	-2.11932000	1.17205000
H	-0.07830100	-5.66625700	0.37795500
H	-0.15186500	-5.38773000	-1.37786100
H	5.91501200	0.38170600	-0.97204000

H	1.83290700	1.60074600	1.49953000
H	3.24745700	4.16452300	-0.89381700
H	3.16745300	4.31390100	0.86415400
H	-1.40541700	4.23232900	2.15274400
H	1.09300200	3.70020900	-2.17082400
H	-3.41695600	4.64728500	-0.94857500
H	-3.51277600	4.64522900	0.83448600
H	-4.34344100	0.14471100	2.24033800
H	-3.83635100	2.49268500	-2.17737500
H	-5.64474500	-1.68092600	-0.73357100
H	-5.43384100	-1.79038700	1.03632900
H	-1.29535700	-3.96043100	1.90398500
H	-3.72180600	-2.43484500	-2.22737100
Li	3.09255300	0.15027300	-1.32722500
Li	1.88896100	-2.28799700	2.48273300
Li	6.34171500	3.84438100	-1.98016800

P5QLi$_4$ (by condensed Fukui function)

E= -2128.608294 hartrees

Symbol	X	Y	Z
C	-4.12639100	-0.59974500	1.17432600
C	-3.17661800	-1.65824400	1.44091200
C	-2.98571200	-2.73338400	0.61201600
C	-3.81808400	-2.86242200	-0.58596800
C	-4.64165100	-1.75067900	-0.92566100
C	-4.79204300	-0.63519800	-0.12638900
C	-1.96789800	-3.81284000	0.90969100
C	-5.39562100	0.61506800	-0.72498200
C	-0.51787400	-3.56176700	0.47927300
C	0.48933400	-3.93224900	1.35826800
C	1.88001300	-3.82868900	1.06719100
C	2.23316800	-3.31917800	-0.22670400
C	1.22115600	-2.93357400	-1.10599900
C	-0.14708700	-3.03386200	-0.80197200
C	3.69097000	-3.21286300	-0.65439600
C	4.14318600	-1.77330200	-0.57867700
C	4.58321500	-1.20046300	0.71303700
C	4.77852600	0.24293100	0.81528600
C	4.65241700	1.06734500	-0.24941500
C	4.36525600	0.48720900	-1.59426400
C	4.10288400	-0.95145600	-1.66126700
C	4.70918900	2.57414400	-0.14996900

C	2.56994500	3.50594800	-1.11078200
C	1.15955700	3.93469400	-0.99275600
C	0.49841600	3.85984500	0.35075200
C	1.23349700	3.47622800	1.41290000
C	2.65754500	3.09059500	1.30723500
C	3.29361000	3.10239700	-0.04884700
C	-0.94315200	4.28841700	0.45368600
C	-2.99888700	1.44060700	-1.29435800
C	-4.27398200	1.62226600	-0.62145000
C	-4.34409900	2.54653100	0.39808200
C	-3.19778300	3.21786600	0.92544900
C	-1.99755500	3.25993800	0.07945900
C	-1.93318600	2.38930100	-0.96938700
O	-2.77980000	0.52143100	-2.15448000
O	-4.34090400	0.30656600	2.05717800
O	2.76192300	-4.19799300	1.94967700
O	4.80852900	-1.91250700	1.72222800
O	0.54207600	4.33718800	-1.97463400
O	-3.75845900	-3.90152400	-1.34242200
O	-1.06928000	-2.67913100	-1.72635400
O	4.34274800	1.20083000	-2.60213900
O	3.29730500	2.77353400	2.30619400
O	-3.20728400	3.64883400	2.13354000
H	-2.60991700	-1.57060700	2.36590300
H	-5.14798300	-1.79775700	-1.88675900
H	-2.33140500	-4.74407300	0.45157600
H	-1.95512700	-3.99852200	1.98866600
H	-6.26911700	0.98150400	-0.17465900
H	-5.69974900	0.41514700	-1.75668700
H	0.23430600	-4.32706000	2.33891800
H	1.47604200	-2.55606100	-2.09458800
H	3.80342700	-3.56145000	-1.68731700
H	4.31047300	-3.85898200	-0.02389200
H	4.98989200	0.62633400	1.80909600
H	3.85014300	-1.33140100	-2.64738200
H	5.18687300	2.97870700	-1.04541600
H	5.27274800	2.86982400	0.73819000
H	0.81833800	3.44066800	2.41723200
H	2.98214700	3.50993400	-2.11542900
H	-1.08639600	5.15891700	-0.20042600
H	-1.15319900	4.60602600	1.47835100
H	-5.27558800	2.66568300	0.94810500
H	-1.05975400	2.34882200	-1.61264900
Li	-2.14567600	-4.08908300	-2.08501300

Li	-1.94826900	-1.08779100	-1.90973200
Li	4.25681100	-3.47802300	2.42715600
Li	-3.87505100	1.93424600	2.67190100

$P5QLi_5$ (by condensed Fukui function)

E= -2136.225021 hartrees

Symbol	X	Y	Z
C	4.12101000	0.42202800	1.17688700
C	3.26439800	1.56422000	1.39570800
C	3.16287500	2.61613600	0.51811100
C	3.98720500	2.62554100	-0.68509500
C	4.72541700	1.44489800	-0.96755600
C	4.79290500	0.35722000	-0.11479100
C	2.23168600	3.78507800	0.75898100
C	5.33190900	-0.95038600	-0.65021000
C	0.77047600	3.60587600	0.34022500
C	-0.22610900	4.09860600	1.20482100
C	-1.61117800	4.02856900	0.93442300
C	-2.03012600	3.40945700	-0.26990400
C	-1.04080600	2.91234900	-1.11696200
C	0.34655300	2.99955400	-0.86827000
C	-3.50083000	3.25600900	-0.65171700
C	-3.99267800	1.82111900	-0.55894300
C	-4.40571700	1.28122200	0.72301100
C	-4.72779900	-0.11221300	0.79351000
C	-4.67394700	-0.94045500	-0.29856100
C	-4.32477300	-0.40409300	-1.61528800
C	-4.00002700	1.00950900	-1.66556300
C	-4.85757400	-2.44115300	-0.19227500
C	-2.74956900	-3.47047100	-1.11925400
C	-1.36483000	-3.94800600	-0.98542700
C	-0.73088400	-3.92922800	0.37392400
C	-1.47200400	-3.54875800	1.43141200
C	-2.88324600	-3.11428100	1.30626900
C	-3.48405400	-3.05700000	-0.06296700
C	0.69368000	-4.41469800	0.49626400
C	2.90972100	-1.69139200	-1.24990300
C	4.16103200	-1.89707000	-0.53210600
C	4.15728500	-2.77828000	0.52239500
C	2.95924500	-3.37732100	1.03451800
C	1.79256800	-3.42942500	0.13820300
C	1.80101300	-2.59855200	-0.94249900

O	2.75013300	-0.78360500	-2.13061600
O	4.25179400	-0.47078100	2.09563400
O	-2.46966800	4.64092800	1.81079200
O	-4.46832500	2.01739400	1.78410100
O	-0.72618800	-4.34971700	-1.95900500
O	3.98949500	3.63276800	-1.49665900
O	1.21176400	2.52114500	-1.79059000
O	-4.28196700	-1.12904700	-2.64139100
O	-3.52897700	-2.82367500	2.30993700
O	2.90586800	-3.73440400	2.26034000
H	2.69085900	1.56223500	2.32079800
H	5.23839100	1.40849200	-1.92560800
H	2.66151900	4.65495100	0.24282200
H	2.23970300	4.03030200	1.82777400
H	6.17468700	-1.33999600	-0.06843400
H	5.66490500	-0.81197500	-1.68308900
H	0.07687400	4.44599200	2.19829800
H	-1.33769600	2.42523100	-2.04290700
H	-3.62691500	3.59785300	-1.68600700
H	-4.11371300	3.91451200	-0.02665400
H	-4.97823000	-0.50589200	1.77495200
H	-3.72399300	1.39436700	-2.64522700
H	-5.34341900	-2.81547500	-1.09669300
H	-5.45837700	-2.69198500	0.68562900
H	-1.07818400	-3.55473800	2.44533300
H	-3.14292100	-3.42184400	-2.12966700
H	0.81208300	-5.28463900	-0.16381600
H	0.87456700	-4.74625800	1.52191800
H	5.06160400	-2.91519200	1.11170600
H	0.95798700	-2.56171600	-1.62514100
Li	2.43282900	3.73316600	-2.34527100
Li	1.94240900	0.84208700	-1.87204300
Li	-3.74477900	3.48393700	2.36463500
Li	3.64782700	-2.02667600	2.75507300
Li	-1.45099600	6.04750900	1.56942100

P5QLi$_6$ (by condensed Fukui function)

E= -2143.830155 hartrees

Symbol	X	Y	Z
C	4.23025300	0.21891300	1.15081400
C	3.44688200	1.41090800	1.35762700
C	3.39451900	2.45344100	0.46114300

C	4.20789400	2.40083500	-0.74433700
C	4.85793400	1.16875900	-1.01952500
C	4.86769800	0.08864100	-0.14914700
C	2.50750000	3.66093700	0.68383500
C	5.30964900	-1.26152600	-0.67348100
C	1.03665600	3.50368900	0.29468800
C	0.05412700	3.98406500	1.18117400
C	-1.33441400	3.93496600	0.91979700
C	-1.76920400	3.34708200	-0.29235300
C	-0.79489800	2.85228600	-1.15853500
C	0.59471600	2.92278800	-0.92190900
C	-3.24111800	3.25963400	-0.68336100
C	-3.84937900	1.86390000	-0.62997200
C	-4.46652100	1.36625700	0.56964100
C	-5.09588600	0.10956600	0.51741400
C	-4.90540300	-0.78897300	-0.52109200
C	-4.24799400	-0.34661800	-1.74303600
C	-3.80190200	1.04189800	-1.73638000
C	-5.08968300	-2.25977700	-0.27569300
C	-3.01897000	-3.48283700	-0.97459600
C	-1.64775900	-3.94944200	-0.82867900
C	-0.96049100	-3.64194500	0.45431900
C	-1.59846000	-2.88519900	1.38094400
C	-2.94694400	-2.36456200	1.19313500
C	-3.68026700	-2.76694600	-0.01153200
C	0.40614800	-4.23963400	0.68028300
C	2.83476900	-1.83932400	-1.22733800
C	4.07961400	-2.12542000	-0.52070700
C	4.02889000	-2.98499900	0.54879500
C	2.79412600	-3.45951500	1.10494400
C	1.59749500	-3.40933900	0.24946400
C	1.65329700	-2.62016500	-0.86059000
O	2.74725100	-0.95616900	-2.14160800
O	4.32288300	-0.66448900	2.08789400
O	-2.18258900	4.54863700	1.80974300
O	-4.33697500	1.95056500	1.78102300
O	-1.06483100	-4.60687600	-1.70703600
O	4.27318700	3.40126200	-1.56845500
O	1.44376800	2.45638200	-1.85860100
O	-4.05427800	-1.10920300	-2.72067100
O	-3.42524900	-1.60619000	2.10035500
O	2.74457300	-3.78745200	2.33930200
H	2.88193600	1.45741300	2.28716300
H	5.35860300	1.08495100	-1.98151700

H	2.95035300	4.49933000	0.12820100
H	2.54251700	3.94356100	1.74319100
H	6.13453300	-1.69766900	-0.09899500
H	5.63274900	-1.16081700	-1.71386300
H	0.37192000	4.30955900	2.17794500
H	-1.10417000	2.39302900	-2.09417900
H	-3.33930600	3.62212900	-1.71348700
H	-3.82739600	3.95714700	-0.07089800
H	-5.63650600	-0.22170300	1.40608800
H	-3.35510000	1.39435300	-2.66366100
H	-5.49687100	-2.77840300	-1.14778200
H	-5.74590400	-2.43600800	0.58451600
H	-1.12732300	-2.63408600	2.32974500
H	-3.51441200	-3.74403100	-1.90285200
H	0.45083300	-5.18404600	0.12094500
H	0.53836100	-4.47253600	1.74084500
H	4.93160200	-3.18206500	1.12357800
H	0.79063900	-2.51623900	-1.51273100
Li	2.73995300	3.58073400	-2.43112200
Li	2.14457600	0.75217800	-1.88373400
Li	-3.61251400	3.51550600	2.16684600
Li	3.64338000	-2.15516700	2.78943600
Li	-1.11432600	5.93118600	1.59887900
Li	-3.76647500	0.16900100	2.30224300

P5QLi$_7$ (by condensed Fukui function)

E= -2151.451751 hartrees

Symbol	X	Y	Z
C	4.07880200	-0.46713000	1.25648900
C	3.70356500	0.91427900	1.42981000
C	3.99768200	1.89920500	0.52077600
C	4.82692500	1.57548300	-0.62814100
C	5.12881300	0.19344500	-0.84741100
C	4.71913600	-0.81872600	-0.01150200
C	3.40469000	3.28832800	0.62752800
C	4.79747200	-2.25541800	-0.49718100
C	1.93206700	3.37512000	0.22586200
C	1.03389400	4.03945300	1.08250100
C	-0.34692700	4.18228300	0.81443000
C	-0.86580500	3.61090700	-0.37461900
C	0.02683900	2.94284000	-1.21161200
C	1.40924400	2.81146100	-0.96413800

C	-2.33093100	3.73775300	-0.77524300
C	-3.19622800	2.48968700	-0.63480800
C	-3.94659200	2.23875900	0.54425400
C	-4.86182700	1.18138300	0.50004000
C	-4.86348400	0.19318500	-0.48729500
C	-4.00624000	0.34415800	-1.62302700
C	-3.28074800	1.57198700	-1.68374500
C	-5.50731300	-1.12533800	-0.09958000
C	-3.93808700	-2.91023400	-0.73754800
C	-2.61115300	-3.44024700	-0.81634800
C	-1.84273400	-3.45788100	0.41330300
C	-2.28209900	-2.67070900	1.45240300
C	-3.44843800	-1.81801500	1.37399700
C	-4.33887200	-2.03233600	0.24075700
C	-0.61872100	-4.34557400	0.52110600
C	2.29351300	-2.39959000	-1.18874300
C	3.42026800	-2.87974800	-0.40858700
C	3.16541900	-3.73570800	0.63250400
C	1.83550100	-3.99175600	1.10677700
C	0.73478900	-3.75253800	0.18154100
C	0.99689000	-2.98860500	-0.92671700
O	2.42248200	-1.46591500	-2.06510700
O	3.80947700	-1.32168000	2.17324400
O	-1.09204600	4.95303600	1.66870200
O	-3.71407800	2.81786200	1.75736800
O	-2.12084600	-3.73609100	-1.97294000
O	5.17863200	2.46879900	-1.49070100
O	2.18160000	2.16367700	-1.86636000
O	-3.85633900	-0.57165700	-2.55134300
O	-3.65026100	-0.92451900	2.28215200
O	1.67086200	-4.24061700	2.35879500
H	3.11491700	1.13869600	2.31696300
H	5.63456300	-0.04529600	-1.78032700
H	4.01400600	3.96623800	0.01470900
H	3.49563100	3.64745000	1.65984100
H	5.48978900	-2.84675800	0.11451400
H	5.17909200	-2.25367800	-1.52336700
H	1.39528000	4.35872900	2.06595100
H	-0.34780000	2.50351300	-2.13317500
H	-2.35998900	4.04013900	-1.82949500
H	-2.78457400	4.56752500	-0.21781900
H	-5.51461600	1.04741300	1.36525400
H	-2.70759100	1.74558700	-2.59356800
H	-6.08187200	-1.57418700	-0.91707400

H	-6.18112800	-0.97481400	0.75095100
H	-1.71020400	-2.61595700	2.37708800
H	-4.58217400	-3.06449000	-1.60214500
H	-0.76695300	-5.20937900	-0.14087500
H	-0.55539000	-4.72904600	1.54380500
H	3.98469300	-4.07081900	1.26876100
H	0.19356700	-2.74977700	-1.61819700
Li	3.71844600	2.92222700	-2.41929500
Li	2.24498300	0.31707200	-1.89090200
Li	-2.66754500	4.17580900	2.09907800
Li	2.81795300	-2.73529500	2.74128700
Li	0.14901200	6.16268300	1.39101300
Li	-3.60261700	0.90475800	2.26904200
Li	-2.94722500	-2.08899000	-2.69664600

P5QLi$_8$ (by condensed Fukui function)

E= -2159.049885 hartrees

Symbol	X	Y	Z
C	3.75627100	-1.64222000	0.97742400
C	3.80018800	-0.28277400	1.44556400
C	4.38734300	0.75087300	0.73827000
C	5.11961600	0.45011000	-0.47493100
C	4.81475800	-0.80958100	-1.06938900
C	4.07680700	-1.80771000	-0.43643700
C	4.16246100	2.20568700	1.10525600
C	3.46386600	-2.91513600	-1.27716400
C	2.82584700	2.75755700	0.59373100
C	1.95284000	3.41215400	1.48762100
C	0.68685300	3.93332900	1.12247600
C	0.27652900	3.80324100	-0.22471700
C	1.14467900	3.17422500	-1.10754800
C	2.38629100	2.61517600	-0.75107600
C	-1.08773900	4.22375100	-0.73136600
C	-2.12169900	3.10195600	-0.76564900
C	-3.24579600	3.12168900	0.09073300
C	-4.29765000	2.26170600	-0.25479800
C	-4.15736700	1.13113900	-1.06564200
C	-2.89759700	0.91781800	-1.70229300
C	-2.00155300	2.02076500	-1.65055500
C	-5.29241000	0.12550500	-0.92247500
C	-4.50884800	-2.19464800	-0.75920800
C	-3.46966700	-3.10446400	-0.39207300

C	-2.88727500	-2.93775900	0.92524000
C	-3.28038900	-1.85797300	1.68972300
C	-4.16281600	-0.82157700	1.22443200
C	-4.74911200	-1.01448500	-0.09104500
C	-1.73520800	-3.82346400	1.31251900
C	0.99231600	-2.12856100	-0.91581600
C	2.03003400	-3.11097500	-0.82221300
C	1.82182100	-4.20288200	0.00716800
C	0.71234400	-4.32879900	0.88978100
C	-0.42930600	-3.49063400	0.60755500
C	-0.23258400	-2.41410600	-0.23020700
O	1.07893700	-0.98747400	-1.61648200
O	3.41870600	-2.60301500	1.76594000
O	-0.03776600	4.62478400	2.06065100
O	-3.31782500	3.77835300	1.27467000
O	-2.93888900	-3.83081600	-1.31733200
O	5.87085200	1.32555000	-1.07381800
O	3.05635400	1.93740900	-1.69367100
O	-2.47647500	-0.22299600	-2.30097600
O	-4.35335900	0.24203600	1.93643500
O	0.81898400	-5.03372300	1.96989500
H	3.32303100	-0.09054700	2.40526000
H	5.15796200	-0.96869900	-2.09243100
H	4.99279900	2.79364500	0.69336900
H	4.19118500	2.33516700	2.19445300
H	3.99526300	-3.86902600	-1.16954200
H	3.53910300	-2.63149600	-2.33444900
H	2.20575800	3.39408600	2.55435600
H	0.86532300	3.07991400	-2.15436400
H	-0.96894900	4.60598800	-1.75356600
H	-1.48425800	5.06654700	-0.15144200
H	-5.24522100	2.40018000	0.26727800
H	-1.14195700	1.99744800	-2.32358200
H	-5.62908900	-0.26484700	-1.88960100
H	-6.14754800	0.62787800	-0.45718800
H	-2.82772000	-1.69340200	2.66589900
H	-4.96301600	-2.35138700	-1.74089700
H	-1.96321600	-4.87322900	1.08964400
H	-1.56224600	-3.77750200	2.39554900
H	2.63273600	-4.91688200	0.14646100
H	-1.05218800	-1.70296000	-0.33803500
Li	4.77272600	2.22115300	-2.12484300
Li	2.60201700	0.10409700	-1.36903500
Li	-1.84057600	4.49012100	1.97952400

Li	2.37181200	-3.95642300	2.29336300
Li	1.47964200	5.49415200	2.30989300
Li	-3.94396100	1.99269400	1.91314000
Li	-2.83385800	-2.06032200	-2.23222900
Li	-0.60679600	-0.19058500	-1.93214400

$P5QLi_9$ (by condensed Fukui function)

E= -2166.644065 hartrees

Symbol	X	Y	Z
C	3.77967200	-1.69460500	1.02004700
C	3.85536400	-0.33461600	1.47312400
C	4.48038300	0.67857300	0.76343300
C	5.21631900	0.35181300	-0.43585700
C	4.88908900	-0.90623700	-1.01710900
C	4.11625100	-1.88173700	-0.38303900
C	4.28041400	2.14071000	1.12004300
C	3.48787000	-2.98184000	-1.22585200
C	2.94878800	2.70675200	0.61382000
C	2.07291200	3.35223200	1.51058600
C	0.81018000	3.88279900	1.14491600
C	0.41063500	3.77695800	-0.20635300
C	1.28052100	3.15516500	-1.09308100
C	2.51526800	2.58058800	-0.73638700
C	-0.94594400	4.21735400	-0.71665700
C	-1.99204400	3.10803800	-0.78566800
C	-3.13041300	3.12581900	0.04969500
C	-4.18866000	2.29196300	-0.33969700
C	-4.05142100	1.17852100	-1.17826900
C	-2.77675300	0.95159000	-1.78343900
C	-1.87143800	2.04442800	-1.69059800
C	-5.22208600	0.20750400	-1.10536700
C	-4.44799200	-2.12401500	-0.88318600
C	-3.39956700	-2.98331500	-0.48038600
C	-2.89989000	-2.78947300	0.86080600
C	-3.39514200	-1.73910000	1.62651300
C	-4.28742900	-0.76419400	1.11887100
C	-4.79151700	-0.94861500	-0.19713100
C	-1.75362900	-3.63892000	1.34379200
C	1.03732500	-2.12057500	-0.92248200
C	2.03800700	-3.13343900	-0.80155800
C	1.77883700	-4.20847500	0.03708900
C	0.65345200	-4.29245800	0.90209800

C	-0.44023500	-3.39636100	0.62215700
C	-0.19885100	-2.34638300	-0.24100100
O	1.18237100	-0.98256200	-1.62995700
O	3.39505500	-2.63685700	1.81577700
O	0.08006200	4.56412900	2.09025900
O	-3.21368900	3.75032500	1.25450600
O	-2.80796400	-3.71952500	-1.37682900
O	5.99357100	1.20931600	-1.04099900
O	3.18195000	1.90504900	-1.67737700
O	-2.35748300	-0.17906500	-2.39028500
O	-4.68236200	0.31363200	1.89339100
O	0.71891700	-5.00742800	1.98458400
H	3.37173900	-0.11879800	2.42489000
H	5.24146900	-1.08741300	-2.03359500
H	5.11507000	2.71183400	0.69330700
H	4.32096000	2.28218700	2.20780900
H	3.98965900	-3.94924200	-1.09757400
H	3.59367600	-2.71005900	-2.28372300
H	2.31920700	3.31700200	2.57878200
H	1.00737500	3.07609500	-2.14271700
H	-0.81487700	4.61767800	-1.73038700
H	-1.34031400	5.05468000	-0.12651000
H	-5.14572000	2.44381700	0.16041400
H	-0.99491700	2.01805400	-2.34012800
H	-5.49233500	-0.20257300	-2.08378400
H	-6.10020600	0.77058700	-0.75465100
H	-3.00858300	-1.58327200	2.63320500
H	-4.84162000	-2.26783900	-1.89192700
H	-1.99237100	-4.70248500	1.21068400
H	-1.60288600	-3.50304800	2.42297800
H	2.55823500	-4.95552300	0.18557700
H	-0.98733500	-1.60008600	-0.35295100
Li	4.91124800	2.10421900	-2.09633400
Li	2.72158500	0.05811700	-1.31685200
Li	-1.71971100	4.43910400	1.96257900
Li	2.29785600	-3.96080800	2.29926700
Li	1.61019000	5.41160600	2.35019800
Li	-3.84000900	1.94966200	1.80640100
Li	-2.67494000	-2.04870200	-2.27948300
Li	-0.48087900	-0.21120400	-2.01434100
Li	-6.24844300	-0.45746900	1.63272300

P5QLi$_{10}$ (by condensed Fukui function)

E= -2174.26431 hartrees

Symbol	X	Y	Z
C	2.23617700	-2.62271600	1.21852900
C	3.26252800	-1.69266100	1.49681400
C	4.42531100	-1.55345400	0.73432400
C	4.69992300	-2.47833300	-0.32004100
C	3.63495900	-3.36656100	-0.63394100
C	2.40385100	-3.41179300	0.04189200
C	5.21204000	-0.25899400	0.81640100
C	1.28695300	-4.20639800	-0.62311400
C	4.35970800	0.90168700	0.30882600
C	4.08644000	1.99885500	1.14911800
C	3.20415100	3.05396900	0.80772500
C	2.58580600	3.01886800	-0.46423300
C	2.87186600	1.94296500	-1.29936700
C	3.70492700	0.86170000	-0.95483100
C	1.58422900	4.05559100	-0.92888100
C	0.11926600	3.65911400	-0.79061700
C	-0.71255400	4.27384600	0.17126500
C	-2.09238500	4.17658900	-0.07038500
C	-2.69507500	3.20472500	-0.86854700
C	-1.83813400	2.31923700	-1.59640300
C	-0.47053400	2.70748900	-1.64485900
C	-4.19776300	3.07895800	-0.66988300
C	-5.03727500	0.78511100	-0.79373000
C	-4.85078300	-0.59525900	-0.58050500
C	-4.37613300	-0.95074500	0.71163400
C	-3.95775400	0.03759600	1.61609200
C	-3.89118200	1.41784400	1.28231100
C	-4.47282300	1.76519200	0.02290300
C	-4.09221800	-2.41625400	0.89424700
C	-0.47199200	-2.29450300	-0.48075100
C	-0.12067700	-3.67291600	-0.42446200
C	-1.09060200	-4.60351600	0.00353800
C	-2.40769400	-4.26186700	0.40811600
C	-2.70219900	-2.86330300	0.45447800
C	-1.75015100	-1.94273900	0.00345000
O	0.39478500	-1.26138600	-0.81695800
O	1.09399200	-2.54805200	1.94976000
O	3.06293100	4.10152300	1.68193000
O	-0.30281400	4.82925600	1.32760600
O	-4.86210000	-1.42958700	-1.61213900
O	5.76478000	-2.39328700	-1.08122200

O	3.78421000	-0.17625800	-1.80263700
O	-2.18592900	1.14970300	-2.19161000
O	-3.26345200	2.28797000	2.06526100
O	-3.29030100	-5.16502200	0.75478900
H	3.08812200	-1.00554400	2.32802400
H	3.76685600	-3.98355300	-1.52283300
H	6.12777400	-0.37627100	0.22437000
H	5.52721100	-0.04315400	1.84579400
H	1.29786800	-5.24665500	-0.27261100
H	1.51697600	-4.26348100	-1.69661900
H	4.46393200	1.96387200	2.17759100
H	2.42211800	1.90449400	-2.28860500
H	1.77765900	4.26068400	-1.99019500
H	1.74943500	5.00755500	-0.40951100
H	-2.73964500	4.82108600	0.52719100
H	0.14900600	2.23267500	-2.40963000
H	-4.73215400	3.10083600	-1.62726900
H	-4.53815600	3.94659600	-0.09221400
H	-3.53802300	-0.25527000	2.57997300
H	-5.45404400	1.08614100	-1.75929100
H	-4.80790500	-2.91200500	0.20251300
H	-4.27739100	-2.74166900	1.93747000
H	-0.82306900	-5.65705300	0.04276400
H	-2.02612800	-0.88971400	0.06123600
Li	5.28444100	-1.11318900	-2.20000300
Li	2.38943700	-1.36094000	-1.18692400
Li	1.38364900	4.78162800	1.85341600
Li	-0.52523300	-3.27421200	1.72157200
Li	4.82314600	4.14339900	1.62254600
Li	-1.98211900	3.47782700	1.99425900
Li	-3.64883600	-0.06460700	-2.25337600
Li	-0.68754600	0.21059800	-1.58200100
Li	-4.92913400	-4.66887800	0.98253300
Li	0.81869400	-0.96908800	1.03495400