Structural Characterization and Bonding Properties of Lithium Naphthalene Radical Anion, $[Li^+(TMEDA)_2][C_{10}H_8^-]$, and Lithium Naphthalene Dianion $[(Li^+TMEDA)_2C_{10}H_8^{-2}]$.

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1. X-ray Analyses

1.1. General

Data collection was performed on a Bruker Smart CCD diffractometer, based on three ω -scan runs (starting $\omega = -34^{\circ}$) at values =0°, 120°, 240° with the detector at $2\theta = -32^{\circ}$. For each of these runs, 606 frames were collected at 0.3° intervals and 30 s per frame. An additional run $=0^{\circ}$ of 100 frames was collected to improve redundancy. The diffraction frames were integrated using the program SAINT¹ and the integrated intensities were corrected for Lorentz-polarisation effects with SADABS.² Structure 1 was solved by direct methods and refined to all 2057 unique F_0^2 by full matrix least squares (SHELX97).³ All the hydrogen atoms were placed at idealised positions and refined as rigid atoms. Final wR2=0.2348 for all data and 127 parameters; R_1 =0.0699 for 1673 F_0 >4 $\sigma(F_0)$. Structure **2** was solved by direct methods and refined to all 3261 unique F_0^2 by full matrix least squares (SHELX97). All the hydrogen atoms were placed at idealised positions and refined as rigid atoms. Final wR2=0.1363 for all data and 158 parameters; R_1 =0.0470 for 2837 F_0 >4 $\sigma(F_0)$. For a complete list of the geometrical parameters as well as further refinement details, please consult the CCDC 695890 and CCDC 695891 cif files, which contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data request/cif.

1.2. Figure S1. Distance lithium-naphthalene anion plane in 1.



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Figure S1. Calculated distance $(5.18 \pm 0.01 \text{ Å})$ between the lithium $[\text{Li}^+(\text{TMEDA})_2]$, and the least-squares mean plane of the anionic naphthalene moiety $[C_{10}H_8^-]$ (blue plane), corresponding to **1**.

1.3. Table S1. Comparison of bond distances of [Li+(TMEDA)2][C10H8•–] (1) with [K+(18-crown-6) (THF)2][C10H8•–] from ref. 5.

Table S1. 0	Comparisor	n of structur	es: bond distances of 1	l				
Bond Dis	tances for	·[Li+(TMEI	DA)2][C10H8•–]	Bond Dis	Bond Distances for [K+(18-crown-6)			
(1) (Angs	troms)			(THF)2][(C10H8•–] (re	f. 5)		
						Absolute		
Object 1	Object2	Length	e.s.d.	Length	e.s.d.	difference		
C7	C7	1.446	0.004	1.449	0.005	0.003		
C7	C8	1.413	0.003	1.406	0.004	0.007		
C8	C9	1.394	0.003	1.394	0.004	0		
C9	C10	1.384	0.004	1.384	0.004	0		
C11	C10	1.397	0.004	1.397	0.004	0		
C11	C7	1.414	0.003	1.412	0.004	0.002		
C8	C7	1.413	0.003	1.406	0.004	0.007		
C8	C9	1.394	0.003	1.394	0.004	0		
C10	C9	1.384	0.004	1.384	0.004	0		
C11	C10	1.397	0.004	1.397	0.004	0		
C7	C11	1.414	0.003	1.412	0.004	0.002		
		Mean of						
		e.s.d.:	0.0034		0.0041			
				Mean of	absolute			

1.4. Table S2. Comparison of bond distances of [Li+(TMEDA)2][C10H8•–] (1)
with [K+([2,2,2]-cryptand)][C10H8•–] from ref. 5.

differences:

0.00136

Table S2. C	Comparisor	n of structur	es: bond distances of	f 1				
Bond Dis	tances for	[Li+(TME	DA)2][C10H8•–] (1))	Bond Distances for [K+([2,2,2]-			
(Angstror	ns)				cryptand)	J[C10H8•–]	
							Absolute	
Object 1	Object2	Length	e.s.d.		Length	e.s.d.	difference	
C7	C7	1.446	0.004		1.455	0.004		0.009
C7	C8	1.413	0.003		1.409	0.003		0.004
C8	C9	1.394	0.003		1.402	0.003		0.008
C9	C10	1.384	0.004		1.373	0.003		0.011
C11	C10	1.397	0.004		1.399	0.003		0.002
C11	C7	1.414	0.003		1.41	0.003		0.004
C8	C7	1.413	0.003		1.409	0.003		0.004
C8	C9	1.394	0.003		1.402	0.003		0.008
C10	C9	1.384	0.004		1.373	0.003		0.011
C11	C10	1.397	0.004		1.399	0.003		0.002
C7	C11	1.414	0.003		1.41	0.003		0.004
		Mean of						
		e.s.d.:	0.0034	_		0.0031		

Mean of absolute	
differences:	0.00609

1.5. Table S3. Comparison of bond angles of [Li+(TMEDA)2][C10H8•–] (1) with [K+(18-crown-6) (THF)2][C10H8•–] from ref. 5.

Table S3.	Comparisor	n of structur	es: bond	angles of	1				
Bond and	gles for					Bond angles for [K+(18-crown-6)			
[Li+(TME	DA)2][C10	OH8•–] (1)	(°)			(THF)2][0	C10H8•–] (ref	. 5) (°)	
	, <u></u>	/				. ,		Absolute	
Object1	Object2	Object3	Angle	e.s.d.		Angle	e.s.d.	difference	
C7	C7	C8	118	0.3		117.5	0.4		0.5
C7	C7	C8	118	0.3		117.5	0.4		0.5
C11	C7	C7	118	0.3		118.5	0.4		0.5
C11	C7	C7	118	0.3		118.5	0.4		0.5
C9	C10	C11	119.6	0.2		119.4	0.3		0.2
C9	C10	C11	119.6	0.2		119.4	0.3		0.2
C8	C9	C10	120.1	0.2		120.3	0.3		0.2
C8	C9	C10	120.1	0.2		120.3	0.3		0.2
C7	C8	C9	122	0.2		121.8	0.3		0.2
C7	C8	C9	122	0.2		121.8	0.3		0.2
C10	C11	C7	122.1	0.2		122.4	0.3		0.3
C10	C11	C7	122.1	0.2		122.4	0.3		0.3
C8	C7	C11	123.9	0.2		123.9	0.3		0
C11	C7	C8	123.9	0.2		123.9	0.3		0
		Mean of	e.s.d.:	0.23			0.33		

0.271

1.6. Table S4. Comparison of bond angles of [Li+(TMEDA)2][C10H8•–] (1) with [K+([2,2,2]-cryptand)][C10H8•–] from ref. 5.

Table S4.	Comparisor	n of structur	res: bond	angles of	1				
Bond and	gles for				Bond an	Bond angles for [K+([2,2,2]-			
[Li+(TME	EDA)2][C10)H8•–] (1)	(°)		cryptand)][C10H8•–] (ref. 5) (°)		
							Absolute		
Object1	Object2	Object3	Angle	e.s.d.	Angle	e.s.d.	difference		
C7	C7	C8	118	0.3	118.1	0.2	0.1		
C7	C7	C8	118	0.3	118.1	0.2	0.1		
C11	C7	C7	118	0.3	118.3	0.2	0.3		
C11	C7	C7	118	0.3	118.3	0.2	0.3		
C9	C10	C11	119.6	0.2	120.1	0.2	0.5		
C9	C10	C11	119.6	0.2	120.1	0.2	0.5		
C8	C9	C10	120.1	0.2	120.5	0.2	0.4		
C8	C9	C10	120.1	0.2	120.5	0.2	0.4		
C7	C8	C9	122	0.2	121.46	0.18	0.54		
C7	C8	C9	122	0.2	121.46	0.18	0.54		
C10	C11	C7	122.1	0.2	121.5	0.18	0.6		
C10	C11	C7	122.1	0.2	121.5	0.18	0.6		
C8	C7	C11	123.9	0.2	123.64	0.17	0.26		
C11	C7	C8	123.9	0.2	123.64	0.17	0.26		

Mean of e.s.d.: 0.23

0.19

0.386

1.7. Table S5. Comparison of bond distances of [(Li+TMEDA)2 C10H8–2] (2) with [(Li+TMEDA)2 C10H8–2] from ref. 8.

Mean of absolute differences:

Table S5. Comparison of structures: bond distances of **2**

Bond distances for [(Li+TMEDA)2 C10H8–2] (2) (°) Bond distances for [(Li+TMEDA)2 C10H8– 2] (ref. 8) (°)

Object	Object2	Longth	aad	Longth	aad	Absolute
		2 1 20	e.s.u.		e.s.u.	
	INZ NI4	2.120	0.002	2.094	0.01	0.033
		2.123	0.002	2.100	0.009	0.01
		2.311	0.002	2.321	0.01	0.01
	010	2.296	0.002	2.265	0.01	0.031
	C10	2.287	0.002	2.257	0.011	0.031
LIT	C11	2.309	0.002	2.327	0.011	0.018
08	09	1.4341	0.0016	1.444	800.0	0.01
C8	C7	1.4214	0.0015	1.432	0.007	0.011
C9	C10	1.3630	0.0017	1.343	0.008	0.02
C10	C11	1.4362	0.0016	1.422	0.008	0.014
C11	C7	1.4142	0.0015	1.412	0.007	0.002
C7	C7	1.4552	0.0019	1.447	0.01	0.008
N2	C6	1.4610	0.0016	1.455	0.008	0.006
N2	C5	1.4634	0.0015	1.459	0.007	0.004
N2	C4	1.4640	0.0014	1.453	0.007	0.011
C4	C3	1.5092	0.0018	1.462	0.009	0.047
N1	C3	1.4690	0.0016	1.478	0.008	0.009
N1	C1	1.4593	0.0016	1.453	0.008	0.006
N1	C2	1.4567	0.0016	1.426	0.008	0.031
Li1	N2	2.128	0.002	2.094	0.01	0.033
Li1	N1	2.123	0.002	2.133	0.009	0.01
Li1	C8	2.311	0.002	2.321	0.01	0.01
Li1	C9	2.296	0.002	2.265	0.01	0.031
Li1	C10	2.287	0.002	2.257	0.011	0.031
Li1	C11	2.309	0.002	2.327	0.011	0.018
C8	C9	1.4341	0.0016	1.444	0.008	0.01
C8	C7	1.4214	0.0015	1.432	0.007	0.011
C9	C10	1.3630	0.0017	1.343	0.008	0.02
C10	C11	1.4362	0.0016	1.422	0.008	0.014
C11	C7	1.4142	0.0015	1.412	0.007	0.002
N2	C6	1.4610	0.0016	1.455	0.008	0.006
N2	C5	1.4634	0.0015	1.459	0.007	0.004
N2	C4	1.4640	0.0014	1.453	0.007	0.011
C4	C3	1.5092	0.0018	1.462	0.009	0.047
N1	C3	1.4690	0.0016	1.478	0.008	0.009
N1	C1	1.4593	0.0016	1.453	0.008	0.006
N1	C2	1.4567	0.0016	1.426	0.008	0.031
	Mean of	e.s.d.:	0.0017		0.0086	

Mean of absolute	
differences:	0.0166

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1.8. Table S6. Comparison of bond angles of [(Li+TMEDA)2 C10H8–2] (2) with [(Li+TMEDA)2 C10H8–2] from ref. 8.

Table S6.	Comparisor	n of structur	es: bond a	angles of	2			
Bond ang	gles for [(L	i+TMEDA)	2		Bond angles for [(Li+TMEDA)2 C10H8–2]			
C10H8-2	2] (2) (°)				(ref. 8) (°)			
Objects	Objecto	Object2	Angle	d	Angle		Absolute	
			Angle	e.s.u.	Angle	e.s.u.		
			85.24	0.08	80.Z	0.4	0.05	
		C9	30.27	0.05	30.7	0.2	0.43	
			13.11	0.07	73.3	0.3	0.47	
C9			34.00	0.05	34.5	0.3	0.1	
010			30.41	0.05	30.1	0.3	0.31	
	60	010	121.24	0.10	119.9	0.5	1.34	
60	010		119.52	0.10	120	0.5	0.48	
010	C10	011	119.32	0.10	119.9	0.5	0.58	
C10	011	07	121.46	0.10	121.3	0.5	0.16	
C11	C7	07	117.84	0.12	118.1	0.6	0.25	
C11	C7	C8	124.61	0.10	124.4	0.5	0.21	
C7	C7	C8	117.55	0.12	117.5	0.6	0.04	
Li1	N2	C4	105.72	0.08	105.6	0.4	0.12	
Li1	N2	C5	104.86	0.09	105.5	0.5	0.64	
Li1	N2	C6	115.81	0.09	115.3	0.5	0.5	
C4	N2	C5	110.92	0.10	111.6	0.5	0.68	
C4	N2	C6	110.04	0.09	111.1	0.5	1.06	
C6	N2	C5	109.36	0.10	107.5	0.5	1.86	
N2	C4	C3	111.32	0.09	114.1	0.6	2.78	
C4	C3	N1	111.99	0.10	114.4	0.5	2.41	
Li1	N1	C3	103.85	0.09	105.3	0.4	1.46	
Li1	N1	C1	106.58	0.09	106	0.5	0.58	
Li1	N1	C2	116.24	0.10	114.9	0.5	1.35	
C3	N1	C2	109.87	0.11	108.9	0.5	0.96	
C3	N1	C1	110.84	0.10	110.6	0.5	0.24	
C2	N1	C1	109.31	0.11	110.7	0.6	1.38	
		Mean of	e.s.d.:	0.092		0.47		
					Moon of abactute			
					differences:		0.786	

1.9. Figure S2. Distance lithium-naphthalene dianion plane in 2.

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Figure S2. Calculated distance $(1.937 \pm 0.006 \text{ Å})$ between the lithium [Li⁺(TMEDA)], and the least-squares mean plane of the anionic naphthalene moiety $[C_{10}H_8^{-2}]$ (blue plane), corresponding to **2**.

2. Computational details

2.1. General

Single point Hartree-Fock (HF), density functional theory (DFT) and second-order Møller-Plesset (MP2) perturbation theory were applied in this study on the experimental X-ray structure **2** after removal of the solvating benzene molecule. The respective calculations were performed with the Gaussian 03 package.⁴ The SCF (self-consistent field Hartree-Fock) convergence criteria were set at 10⁻⁸ a.u., and a pruned grid having 99 radial shells and 590 angular points per shell, was used in all cases. Calculations at the HF, DFT⁵ using the B3LYP exchange-correlation functional,⁶ and MP2⁷ levels of theory were performed using the corresponding basis sets⁸ as stated in Table 1. Natural Atomic Orbital and Natural Population Analysis (NPA) were performed using the NBO program Version 3.1.⁹ The corresponding summaries of the NPA including natural atomic charges and natural electron configuration, followed by the summary of the corresponding *ab initio* or DFT calculation, are listed below.

2.2. HF/6-31+G(d,p)

Atom Natural Wateres Core Valence Rydberg Total Li 1 0.89127 1.99919 0.08374 0.02580 2.10873 N 2 -0.64335 1.99950 5.62367 0.022607 7.64335 C 3 -0.34000 1.99950 4.32667 0.01343 6.34000 H 4 0.20135 0.00000 0.80827 0.00144 0.82971 H 6 0.17115 0.00000 0.82744 0.00144 0.82971 H 8 0.16610 0.00000 0.8201 0.00166 0.79884 H 10 0.2012 0.00000 0.80201 0.00166 0.8365 H 13 0.19638 0.00000 0.80571 0.00161 0.8072 H 15 0.19278 0.00000 0.818317 0.01671 6.19297 H 16 0.18380 0.00000 0.81671 0.00149 0.81620 N			No burne 1	Natural Population						
Li 1 0.89127 1.99919 0.08374 0.02580 2.10873 N 2 -0.64935 1.99961 5.62367 0.02607 7.64935 C 3 -0.34000 1.9950 4.32667 0.01383 6.34000 H 4 0.20135 0.00000 0.79634 0.00231 0.79865 H 5 0.19029 0.00000 0.80274 0.00144 0.80971 H 6 0.17115 0.00000 0.82744 0.00141 0.82885 C 7 -0.33221 1.99951 4.32024 0.01346 6.3321 H 8 0.16610 0.00000 0.8201 0.00161 0.83362 H 10 0.2012 0.00000 0.8201 0.00161 0.83362 H 10 0.2012 0.00000 0.8201 0.00164 0.83190 H 12 0.19638 0.00000 0.8009 0.00149 0.81365 C 11 -0.17004 1.99938 4.15370 0.01666 6.17004 H 12 0.1942 0.00000 0.8009 0.00149 0.81981 C 14 -0.16927 1.99339 4.15317 0.01671 6.16927 H 15 0.19278 0.00000 0.81815 0.00144 0.8190 N 17 -0.65432 1.99961 5.62975 0.02486 7.8432 C 18 -0.33811 1.99948 4.32501 0.01367 6.33811 H 19 0.16705 0.00000 0.81167 0.00151 0.80722 H 16 0.18380 0.00000 0.81167 0.00154 0.81295 H 20 0.22421 0.00000 0.81167 0.00139 0.81295 H 21 0.18694 0.00000 0.81267 0.00139 0.81295 H 22 0.16705 0.00000 0.81267 0.00139 0.81295 H 22 0.16743 0.00000 0.81267 0.00139 0.81295 C 22 -0.33462 1.99949 4.32166 0.01348 6.33811 H 19 0.16705 0.00000 0.81202 0.00125 0.81327 H 21 0.18694 0.00000 0.81267 0.00139 0.81295 H 22 0.1674 0.00000 0.77927 0.00180 0.78107 H 22 0.1674 1.99926 4.52237 0.02496 7.98126 C 22 -0.33462 1.99949 4.32166 0.01348 6.28760 C 29 -0.28716 1.99931 4.25542 0.03244 6.28716 H 23 0.18673 0.00000 0.81267 0.00134 6.81362 C 29 -0.28716 1.99931 4.25542 0.03244 6.28716 H 30 0.18130 0.00000 0.81067 0.00134 0.81362 C 31 -0.10196 1.99932 4.26986 0.03278 6.30195 C 31 -0.54347 1.99925 4.50576 0.03847 6.54347 H 34 0.18806 0.00000 0.81027 0.00186 0.81060 C 29 -0.28716 1.99931 4.25542 0.03244 6.28716 H 30 0.18278 0.00000 0.8107 0.03244 6.54347 H 34 0.18806 0.00000 0.8107 0.03246 6.33011 H 34 0.18806 0.00000 0.8107 0.03246 6.3301 H 34 0.19638 0.00000 0.8107 0.03246 6.3301 H 34 0.19638 0.00000 0.8107 0.03246 6.3301 H 34 0.19638 0.00000 0.8077 0.00144 0.82885 C 37 -0.73400 1.99950 4.32667 0.03847 6.54347 H 34 0.19638 0.00000 0.80571 0.00148 0.80390 H 33 0.19638 0.00000 0.80571 0.00148	Atom	No	Charge	Core	Valence	Rydberg	Total			
N 2 -0.64935 1.99961 5.62367 0.02607 7.64935 C 3 -0.34000 1.99950 4.32667 0.01183 6.34000 H 5 0.19029 0.00000 0.8827 0.01444 0.80971 H 6 0.17115 0.00000 0.88244 0.00141 0.82985 C 7 -0.33321 1.99951 4.32024 0.01346 6.33321 H 8 0.16610 0.00000 0.80201 0.00161 0.80362 H 10 0.2012 0.00000 0.80201 0.0166 6.17004 H 12 0.19842 0.00000 0.81093 0.00146 0.81581 C 14 0.16277 1.99939 4.15317 0.01671 6.16927 H 15 0.13278 0.00000 0.81571 0.01671 6.16927 H 15 0.16705 0.00000 0.81571 0.01671 6.16927 H <	Li	1	0.89127	1.99919	0.08374	0.02580	2.10873			
C 3 -0.34000 1.99950 4.32667 0.01383 6.34000 H 4 0.20135 0.00000 0.82744 0.00144 0.80971 H 6 0.17115 0.00000 0.82744 0.01346 6.33321 H 8 0.16610 0.00000 0.83056 0.001346 6.83321 H 8 0.16610 0.00000 0.83056 0.00140 0.80362 H 9 0.19638 0.00000 0.83056 0.0166 0.79988 C 11 -0.17004 1.99938 4.15370 0.01696 6.17004 H 13 0.18019 0.00000 0.81835 0.00149 0.80158 H 13 0.18019 0.00000 0.81835 0.00149 0.81072 H 16 0.19278 0.00000 0.81471 0.0166 6.73841 H 19 0.16705 0.00000 0.81471 0.01362 6.33462 H	Ν	2	-0.64935	1.99961	5.62367	0.02607	7.64935			
H 4 0.20135 0.00000 0.79634 0.00231 0.79665 H 5 0.19029 0.00000 0.80274 0.00141 0.82785 H 6 0.17115 0.00000 0.80274 0.01346 0.83321 H 8 0.16610 0.00000 0.80201 0.00161 0.80366 H 9 0.19638 0.00000 0.80201 0.00166 0.79981 C 11 0.17004 1.99934 4.15370 0.01696 6.17004 H 12 0.19842 0.00000 0.8009 0.00146 0.81581 C 14 0.16927 1.99939 4.15317 0.01671 6.16927 H 15 0.19278 0.00000 0.80571 0.0149 0.81520 N 17 -0.65432 1.99941 4.32501 0.01671 6.16927 H 20 0.22421 0.00000 0.81202 0.0139 0.832265 H <	С	3	-0.34000	1.99950	4.32667	0.01383	6.34000			
H 5 0.19029 0.00000 0.8827 0.00144 0.80971 H 6 0.17115 0.00000 0.82744 0.00146 6.33321 H 8 0.16810 0.00000 0.83056 0.001346 6.33321 H 8 0.16810 0.00000 0.83051 0.00161 0.83052 H 10 0.20012 0.00000 0.83050 0.00166 0.79988 C 11 -0.17004 1.99938 4.15370 0.01696 0.80971 H 13 0.18019 0.00000 0.81835 0.00149 0.8158 H 13 0.19278 0.00000 0.81471 0.01490 0.81620 N 17 -0.65432 1.99948 4.32501 0.01362 6.33811 H 19 0.16705 0.00000 0.81262 0.00171 0.77579 H 21 0.16673 0.00000 0.81167 0.01390 0.83295 C	Н	4	0.20135	0.00000	0.79634	0.00231	0.79865			
H 6 0.17115 0.00000 0.82744 0.01146 6.32885 C 7 -0.3321 1.99951 4.32024 0.01346 6.33211 H 8 0.16810 0.00000 0.83056 0.00134 0.83321 H 9 0.19638 0.00000 0.80201 0.00166 0.79988 C 11 -0.17004 1.99938 4.15370 0.01696 6.17004 H 12 0.19842 0.00000 0.8185 0.00146 0.81981 C 14 -0.16927 1.99939 4.15317 0.01671 6.16927 H 15 0.19278 0.00000 0.81571 0.0146 0.81981 C 14 -0.165432 1.99944 4.32501 0.01362 6.33811 H 19 0.16705 0.00000 0.81205 0.00171 0.77579 H 20 0.22421 0.00000 0.81202 0.00171 0.77579 H	Н	5	0.19029	0.00000	0.80827	0.00144	0.80971			
C 7 -0.33321 1.99951 4.32024 0.01346 6.33321 H 8 0.166810 0.00000 0.83056 0.00134 0.83190 H 9 0.19638 0.00000 0.83021 0.00161 0.83622 H 10 0.20012 0.00000 0.80201 0.001696 6.17004 H 12 0.19842 0.00000 0.81357 0.01646 0.81981 C 14 0.16927 1.99394 4.15317 0.01671 6.16927 H 15 0.19278 0.00000 0.8171 0.00151 0.80722 H 16 0.18380 0.00000 0.81471 0.00149 0.81620 N 7 0.65432 1.99948 4.32501 0.01362 6.33811 H 9 0.18705 0.00000 0.81267 0.01348 6.33462 H 20 0.22421 0.00000 0.81202 0.00131 0.83462 H	Н	6	0.17115	0.00000	0.82744	0.00141	0.82885			
H 8 0.16810 0.00000 0.83056 0.00141 0.83120 H 9 0.19638 0.00000 0.8021 0.00161 0.8362 H 10 0.2012 0.0000 0.79821 0.00166 0.79988 C 11 -0.17004 1.9938 4.15370 0.01666 6.17004 H 12 0.18842 0.00000 0.81835 0.00146 0.81981 C 14 -0.16927 1.99393 4.15317 0.01671 6.16927 H 15 0.19278 0.00000 0.81835 0.00149 0.81620 N 17 -0.65432 1.99961 5.62975 0.02496 7.65432 C 18 0.33811 1.99948 4.32161 0.0139 0.83295 H 20 0.22421 0.00000 0.81167 0.00139 0.83262 H 23 0.18673 0.00000 0.81262 0.03246 6.33462 H	С	7	-0.33321	1.99951	4.32024	0.01346	6.33321			
H 9 0.19638 0.0000 0.80201 0.00161 0.80362 H 10 0.20012 0.0000 0.79821 0.00166 0.79988 C 11 -0.17004 1.99938 4.15370 0.01696 6.17004 H 12 0.18019 0.00000 0.8009 0.00149 0.80158 H 13 0.18019 0.00000 0.81351 0.001671 6.16927 H 15 0.19278 0.00000 0.80571 0.00151 0.80722 H 16 0.18380 0.00000 0.81471 0.0149 0.81620 N 17 -0.65432 1.99941 4.32501 0.0139 0.83295 H 20 0.22421 0.00000 0.81167 0.00171 0.77579 H 21 0.18694 0.00000 0.81202 0.00139 0.81306 C 2.6 0.16574 0.00000 0.83295 0.00131 0.83426 C	Н	8	0.16810	0.0000	0.83056	0.00134	0.83190			
H 10 0.20012 0.00000 0.79821 0.00166 0.79988 C 11 -0.17004 1.99938 4.15370 0.01696 6.17004 H 12 0.18019 0.0000 0.80099 0.00149 0.80158 C 14 -0.16927 1.99394 4.15317 0.01671 6.16927 H 15 0.19278 0.00000 0.80571 0.00149 0.81620 N 17 -0.65432 1.99961 5.62975 0.02496 7.65432 C 18 -0.33811 1.99948 4.32501 0.01362 6.33811 H 19 0.16705 0.00000 0.81167 0.00139 0.83295 H 20 0.22421 0.00000 0.81167 0.00139 0.83462 H 21 0.18694 0.00000 0.81202 0.00131 0.83462 H 24 0.21893 0.00000 0.81202 0.00130 0.81326 C	Н	9	0.19638	0.0000	0.80201	0.00161	0.80362			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	H	10	0.20012	0.00000	0.79821	0.00166	0.79988			
H 12 0.19842 0.0000 0.8009 0.00149 0.80158 H 13 0.18019 0.0000 0.81835 0.00146 0.81981 C 14 -0.16927 1.99939 4.15317 0.01671 6.16927 H 15 0.12778 0.0000 0.80571 0.00151 0.80722 H 16 0.18380 0.0000 0.8157 0.02496 7.65432 C 18 -0.33811 1.99948 4.32501 0.01362 6.33811 H 19 0.16705 0.00000 0.81167 0.00171 0.77579 H 21 0.18674 0.00000 0.81167 0.00125 0.81327 H 24 0.21893 0.00000 0.81202 0.00131 0.84265 C 26 0.1897 0.99909 3.95395 0.02801 5.98105 C 27 -0.56242 1.99924 4.25237 0.4078 6.56242 H	С	11	-0.17004	1.99938	4.15370	0.01696	6.17004			
H 13 0.18019 0.00000 0.81835 0.00146 0.81981 C 14 -0.16927 1.99939 4.15317 0.00151 6.16927 H 15 0.19278 0.00000 0.81471 0.00149 0.81620 N 17 -0.65432 1.99961 5.62975 0.02496 7.65432 C 18 -0.33811 1.99948 4.32501 0.01326 6.33811 H 19 0.16705 0.00000 0.81167 0.00139 0.81295 H 20 0.22421 0.00000 0.81167 0.00139 0.81306 C 22 -0.33462 1.99949 4.32166 0.01348 6.34622 H 23 0.18673 0.00000 0.81207 0.00125 0.81327 H 24 0.21893 0.00000 0.82295 0.00131 0.84266 C 26 0.16574 0.00000 0.83295 0.00171 0.81327 H	Н	12	0.19842	0.00000	0.80009	0.00149	0.80158			
C 14 -0.16927 1.99939 4.15317 0.01671 6.16927 H 15 0.19278 0.00000 0.80571 0.00151 0.80722 H 16 0.18380 0.00000 0.81471 0.00149 0.81620 N 17 -0.65432 1.99961 5.62975 0.02496 7.65432 C 18 -0.33811 1.99948 4.32501 0.01362 6.33811 H 19 0.16705 0.00000 0.81156 0.00139 0.83295 H 20 0.22421 0.00000 0.81167 0.00139 0.83295 H 21 0.18694 0.00000 0.81120 0.00139 0.81367 C 22 -0.33462 1.99949 4.32166 0.01348 6.33462 H 23 0.18673 0.00000 0.81202 0.00125 0.81327 H 24 0.21893 0.00000 0.77927 0.00180 0.78107 H 25 0.16574 0.00000 0.83295 0.00131 0.83426 C 27 -0.56242 1.99926 4.52237 0.04078 6.56242 H 28 0.18940 0.0000 0.81693 0.00177 0.81870 C 29 -0.28716 1.99931 4.25542 0.32244 6.28716 H 30 0.18130 0.00000 0.81693 0.00177 0.81870 C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00177 0.81870 C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00177 0.81870 C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00177 0.81870 C 31 -0.30196 1.99931 4.25542 0.03244 6.28716 H 30 0.18130 0.00000 0.81548 0.00177 0.81870 C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00177 0.81870 C 33 -0.54347 1.99925 4.50576 0.03847 6.54347 H 34 0.18806 0.00000 0.81022 0.00192 0.81194 Li 35 0.89127 1.99919 0.08374 0.02580 2.10873 N 36 -0.64935 1.99951 4.32667 0.01383 6.34000 H 38 0.20135 0.00000 0.80827 0.00144 0.80971 H 40 0.17115 0.00000 0.80827 0.00144 0.80971 H 40 0.17115 0.00000 0.80827 0.00144 0.80971 H 40 0.17115 0.00000 0.80827 0.00144 0.80971 H 40 0.16810 0.00000 0.80827 0.00144 0.80971 H 40 0.16810 0.00000 0.80827 0.00144 0.80971 H 40 0.16810 0.00000 0.80156 0.00134 0.83190 H 43 0.19638 0.00000 0.80257 0.00144 0.80362 H 44 0.20012 0.00000 0.80257 0.00144 0.80362 H 44 0.20012 0.00000 0.80571 0.00151 0.80722 H 50 0.18380 0.00000 0.80577 0.02146 0.43381 C 48 -0.16927 1.99939 4.15317 0.01666 0.79988 C 45 -0.17004 1.99938 4.15370 0.01661 0.80362 H 50 0.18380 0.00000 0.81471 0.00149 0.81620 N 51 -0	Н	13	0.18019	0.00000	0.81835	0.00146	0.81981			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	14	-0.16927	1.99939	4.15317	0.01671	6.16927			
H 16 0.18380 0.00000 0.81471 0.00149 0.81620 N 17 -0.65432 1.99948 4.32501 0.01362 6.33811 H 19 0.16705 0.00000 0.83156 0.00171 0.77579 H 20 0.22421 0.00000 0.81167 0.00139 0.81306 C 22 -0.33462 1.99949 4.32166 0.01348 6.33462 H 23 0.18673 0.00000 0.81202 0.00125 0.81327 H 24 0.21893 0.00000 0.81202 0.00180 0.78107 H 25 0.16574 0.00000 0.82235 0.00131 0.83426 C 26 0.01895 1.99926 4.52237 0.04078 6.56242 H 28 0.18240 0.00000 0.81693 0.0177 0.81870 C 29 -0.28716 1.99932 4.26586 0.03278 6.30196 H	H	15	0.19278	0.00000	0.80571	0.00151	0.80722			
N 17 -0.65432 1.99961 5.62975 0.02496 7.65432 C 18 -0.33811 1.99948 4.32501 0.01362 6.33811 H 19 0.16705 0.0000 0.81167 0.00139 0.83295 H 20 0.22421 0.00000 0.81167 0.00139 0.83362 H 21 0.18673 0.00000 0.81202 0.00125 0.81327 H 23 0.18673 0.00000 0.81202 0.00125 0.81327 H 24 0.21893 0.00000 0.81202 0.00130 0.78107 H 25 0.16574 0.00000 0.83295 0.02801 5.98105 C 27 -0.56242 1.99926 4.52237 0.04078 6.56242 H 28 0.18940 0.00000 0.81673 0.00177 0.81870 C 27 -0.56242 1.999131 4.25542 0.03244 6.28716 H	H	16	0.18380	0.00000	0.81471	0.00149	0.81620			
C 18 -0.33811 1.99948 4.32501 0.01362 6.33811 H 19 0.16705 0.00000 0.83156 0.00139 0.83295 H 20 0.22421 0.00000 0.81167 0.00139 0.81306 C 22 -0.33462 1.99949 4.32166 0.01348 6.33462 H 24 0.18673 0.00000 0.81167 0.00125 0.81327 H 24 0.21893 0.00000 0.83295 0.00131 0.83426 C 26 0.16574 0.00000 0.83295 0.02801 5.98105 C 27 -0.56242 1.99926 4.52337 0.04078 6.56242 H 28 0.18940 0.00000 0.81874 0.00186 0.81060 C 27 -0.56242 1.99931 4.25542 0.03278 6.30196 H 30 0.18130 0.00000 0.81548 0.00177 0.81702 C	N	17	-0.65432	1.99961	5.62975	0.02496	7.65432			
H 19 0.16705 0.00000 0.83156 0.00139 0.83295 H 20 0.22421 0.00000 0.77408 0.00171 0.77579 H 21 0.18694 0.00000 0.81167 0.00139 0.81306 C 22 -0.33462 1.99949 4.32166 0.01348 6.33462 H 23 0.18673 0.00000 0.81202 0.00125 0.81327 H 24 0.21893 0.00000 0.77927 0.00180 0.78107 H 25 0.16574 0.00000 0.83295 0.00131 0.83426 C 26 0.01895 1.99909 3.95395 0.02801 5.98105 C 27 -0.56242 1.99926 4.52237 0.00186 0.81660 C 29 -0.28716 1.99931 4.25542 0.03244 6.28716 H 30 0.18130 0.00000 0.81633 0.00175 0.81722 C 33 -0.54347 1.99925 4.50576 0.03247 6.54347	C	18	-0.33811	1.99948	4.32501	0.01362	6.33811			
H 20 0.22421 0.00000 0.7448 0.00171 0.77579 H 21 0.18694 0.00000 0.81167 0.00139 0.81366 C 22 -0.33462 1.99949 4.32166 0.01348 6.33462 H 23 0.18673 0.00000 0.81202 0.00125 0.81327 H 24 0.21893 0.00000 0.77927 0.00180 0.78107 H 25 0.16574 0.00000 0.83255 0.00131 0.83426 C 26 0.01895 1.99909 3.95395 0.02801 5.98105 C 27 -0.56242 1.99926 4.52337 0.04078 6.56242 H 28 0.18940 0.00000 0.81693 0.00177 0.81870 C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00175 0.81722 C 33 -0.54347 1.99925 4.50576 0.03847 6.54347	H	19	0.16705	0.00000	0.83156	0.00139	0.83295			
H 21 0.18694 0.0000 0.81167 0.00139 0.81368 C 22 -0.33462 1.99949 4.32166 0.01348 6.33462 H 23 0.18673 0.00000 0.81202 0.00125 0.81327 H 24 0.21893 0.00000 0.83295 0.00131 0.83426 C 26 0.01895 1.99909 3.95395 0.02801 5.98105 C 26 0.1895 1.99909 3.95395 0.02801 5.98105 C 27 -0.56242 1.99926 4.52237 0.04078 6.56242 H 28 0.18940 0.00000 0.81074 0.00186 0.81060 C 29 -0.28716 1.99931 4.25542 0.03244 6.28716 H 30 0.18130 0.00000 0.81693 0.00177 0.81870 C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.8174 0.02580 2.10873 <	H	20	0.22421	0.00000	0.77408	0.00171	0.77579			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	H	21	0.18694	0.00000	0.81167	0.00139	0.81306			
H 23 0.18873 0.00000 0.77927 0.00125 0.81227 H 24 0.21893 0.00000 0.77927 0.00130 0.83426 C 26 0.01895 1.99909 3.95395 0.02801 5.98105 C 27 -0.56242 1.99926 4.52237 0.04078 6.56242 H 28 0.18940 0.00000 0.80874 0.00186 0.81060 C 29 -0.28716 1.99931 4.25542 0.03244 6.28716 H 30 0.18130 0.00000 0.81693 0.00177 0.81870 C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00175 0.81722 C 33 -0.54347 1.99925 4.50576 0.03847 6.54347 H 34 0.18205 1.99961 5.62367 0.02580 2.10873 N 36 -0.64935 1.99951 4.32667 0.01383 6.34000	C II	22	-0.33462	1.99949	4.32166	0.01348	6.33462			
H 24 0.21893 0.00000 0.77927 0.00130 0.74107 H 25 0.16574 0.00000 0.83295 0.00131 0.83426 C 26 0.01895 1.99909 3.95395 0.02801 5.98105 C 27 -0.56242 1.99926 4.52237 0.04078 6.56242 H 28 0.18940 0.00000 0.80874 0.00186 0.81060 C 29 -0.28716 1.99931 4.25542 0.03244 6.28716 H 30 0.18130 0.00000 0.81693 0.00177 0.81870 C 31 -0.30196 1.99932 4.266986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00175 0.81722 C 33 -0.54347 1.99925 4.50576 0.03847 6.54347 H 34 0.18935 1.99961 5.62367 0.02580 2.10873 N 36 -0.64935 1.99950 4.32667 0.01341 0.80271	H	∠3 24	0.18673	0.00000	0.81202	0.00125	0.81327			
H 23 0.16374 0.00000 0.03233 0.00131 0.03426 C 26 0.01895 1.99909 3.95395 0.02801 5.98105 C 27 -0.56242 1.99926 4.52237 0.04078 6.56242 H 28 0.18940 0.00000 0.80874 0.00186 0.81060 C 29 -0.28716 1.99931 4.25542 0.03244 6.28716 H 30 0.18130 0.00000 0.81693 0.00177 0.81870 C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00175 0.81722 C 33 -0.54347 1.99925 4.50576 0.03847 6.54347 H 34 0.18806 0.00000 0.81002 0.00192 0.81194 Li 35 0.89127 1.99919 0.08277 0.02607 7.64935 C 37 -0.34000 1.99950 4.32667 0.01343 6.33201	п u	24	0.21893	0.00000	0.77927	0.00180	0.78107			
C 20 0.01093 1.99909 3.99933 0.04078 6.56242 H 28 0.18940 0.00000 0.80874 0.00186 0.81060 C 29 -0.28716 1.99931 4.25542 0.03244 6.28716 H 30 0.18130 0.00000 0.81693 0.00177 0.81870 C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00175 0.81722 C 33 -0.54347 1.99925 4.50576 0.03847 6.54347 H 34 0.18806 0.00000 0.81002 0.00192 0.81194 Li 35 0.89127 1.99919 0.08374 0.02580 2.10873 N 36 -0.64935 1.99961 5.62367 0.02607 7.64935 C 37 -0.34000 1.99950 4.32667 0.01383 6.34000 H 38 0.20135 0.00000 0.88027 0.00144 0.80971 H 40 0.17115 0.00000 0.82744 0.00141 0.82885 C 41 -0.33321 1.99951 4.32024 0.01346 6.33321 H 42 0.16810 0.00000 0.83056 0.00134 0.83190 H 43 0.19638 0.00000 0.80201 0.0161 0.80362 H 44 0.20012 0.00000 0.80201 0.00161 0.80362 H 44 0.20012 0.00000 0.810201 0.00166 0.79988 C 45 -0.17004 1.99938 4.15377 0.01666 6.17004 H 46 0.19842 0.00000 0.810201 0.00149 0.80158 H 47 0.18019 0.00000 0.80201 0.0166 0.79988 C 45 -0.17004 1.99938 4.15317 0.01666 6.17004 H 46 0.19842 0.00000 0.810201 0.00149 0.80158 H 47 0.18019 0.00000 0.80201 0.00149 0.80158 H 47 0.18019 0.00000 0.80201 0.0166 0.79988 C 48 -0.16927 1.99939 4.15317 0.01671 6.16927 H 49 0.19278 0.00000 0.810571 0.00149 0.80158 H 47 0.18019 0.00000 0.810571 0.00149 0.81620 N 51 -0.65432 1.99961 5.62975 0.02496 7.65432 C 52 -0.33811 1.99948 4.32501 0.01362 6.33811	пС	25	0.10574	1 99909	2 95395	0.00131	0.03420 5 00105			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	20	-0 56242	1 99926	4 52237	0.02801	5.90105			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	с u	29	0 18940	0 00000	0 80874	0.04078	0.30242			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C II	29	-0 28716	1 99931	4 25542	0 03244	6 28716			
C 31 -0.30196 1.99932 4.26986 0.03278 6.30196 H 32 0.18278 0.00000 0.81548 0.00175 0.81722 C 33 -0.54347 1.99925 4.50576 0.03847 6.54347 H 34 0.18806 0.00000 0.81002 0.00192 0.81194 Li 35 0.89127 1.99919 0.08374 0.02580 2.10873 N 36 -0.64935 1.99961 5.62367 0.02607 7.64935 C 37 -0.34000 1.99950 4.32667 0.01383 6.34000 H 38 0.20135 0.00000 0.79634 0.00231 0.79865 H 39 0.19029 0.00000 0.80827 0.00141 0.82885 C 41 -0.33321 1.99951 4.32024 0.0141 0.82885 C 41 -0.6810 0.00000 0.80201 0.00161 0.80362 H 42 0.16810 0.00000 0.80201 0.00161 0.80362	н	30	0.18130	0.00000	0.81693	0.00177	0.81870			
H320.182780.000000.815480.001750.81722C33-0.543471.999254.505760.038476.54347H340.188060.000000.810020.001920.81194Li350.891271.999190.083740.025802.10873N36-0.649351.999615.623670.026077.64935C37-0.340001.999504.326670.013836.34000H380.201350.000000.796340.002310.79865H390.190290.000000.808270.001440.80971H400.171150.000000.827440.001410.82885C41-0.333211.999514.320240.013466.33321H420.168100.000000.802010.001610.80362H440.200120.000000.802010.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.800090.001490.80158H470.180190.000000.805710.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999	C	31	-0.30196	1.99932	4.26986	0.03278	6.30196			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	32	0.18278	0.00000	0.81548	0.00175	0.81722			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	33	-0.54347	1.99925	4.50576	0.03847	6.54347			
Li 35 0.89127 1.99919 0.08374 0.02580 2.10873 N 36 -0.64935 1.99961 5.62367 0.02607 7.64935 C 37 -0.34000 1.99950 4.32667 0.01383 6.34000 H 38 0.20135 0.00000 0.79634 0.00231 0.79865 H 39 0.19029 0.00000 0.80827 0.00144 0.80971 H 40 0.17115 0.00000 0.82744 0.00141 0.82885 C 41 -0.33321 1.99951 4.32024 0.01346 6.33321 H 42 0.16810 0.00000 0.83056 0.00134 0.83190 H 43 0.19638 0.00000 0.80201 0.00161 0.80362 H 44 0.20012 0.00000 0.79821 0.00166 0.79988 C 45 -0.17004 1.99938 4.15370 0.01696 6.17004 H 46 0.19842 0.00000 0.81835 0.00149 0.80158 H 47 0.18019 0.00000 0.81835 0.00146 0.81981 C 48 -0.16927 1.99939 4.15317 0.01671 6.16927 H 49 0.19278 0.00000 0.80571 0.00151 0.80722 H 50 0.18380 0.00000 0.81471 0.00149 0.81620 N 51 -0.65432 1.99961 5.62975 0.02496 7.65432 C 52 -0.33811 1.99948 4.32501 0.01362 6.33811	Н	34	0.18806	0.00000	0.81002	0.00192	0.81194			
N36-0.649351.999615.623670.026077.64935C37-0.340001.999504.326670.013836.34000H380.201350.000000.796340.002310.79865H390.190290.000000.808270.001440.80971H400.171150.000000.827440.001410.82885C41-0.333211.999514.320240.013466.33321H420.168100.000000.802010.001610.80362H430.196380.000000.802010.001610.80362H440.200120.000000.798210.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432L99484.325010.01362633811	Li	35	0.89127	1.99919	0.08374	0.02580	2.10873			
C37-0.340001.999504.326670.013836.34000H380.201350.000000.796340.002310.79865H390.190290.000000.808270.001440.80971H400.171150.000000.827440.001410.82885C41-0.333211.999514.320240.013466.33321H420.168100.000000.830560.001340.83190H430.196380.000000.802010.001610.80362H440.200120.000000.798210.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.800090.001490.80158H470.180190.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999484.325010.013626.33811	Ν	36	-0.64935	1.99961	5.62367	0.02607	7.64935			
H380.201350.000000.796340.002310.79865H390.190290.000000.808270.001440.80971H400.171150.000000.827440.001410.82885C41-0.333211.999514.320240.013466.33321H420.168100.000000.830560.001340.83190H430.196380.000000.802010.001610.80362H440.200120.000000.798210.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.800090.001490.80158H470.180190.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999484.325010.013626.33811	С	37	-0.34000	1.99950	4.32667	0.01383	6.34000			
H390.190290.000000.808270.001440.80971H400.171150.000000.827440.001410.82885C41-0.333211.999514.320240.013466.33321H420.168100.000000.830560.001340.83190H430.196380.000000.802010.001610.80362H440.200120.000000.798210.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.800090.001490.80158H470.180190.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999484.325010.013626.33811	Н	38	0.20135	0.0000	0.79634	0.00231	0.79865			
H400.171150.000000.827440.001410.82885C41-0.333211.999514.320240.013466.33321H420.168100.000000.830560.001340.83190H430.196380.000000.802010.001610.80362H440.200120.000000.798210.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.800090.001490.80158H470.180190.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999484.325010.013626.33811	Н	39	0.19029	0.0000	0.80827	0.00144	0.80971			
C41-0.333211.999514.320240.013466.33321H420.168100.000000.830560.001340.83190H430.196380.000000.802010.001610.80362H440.200120.000000.798210.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.800090.001490.80158H470.180190.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999484.325010.013626.33811	Η	40	0.17115	0.00000	0.82744	0.00141	0.82885			
H420.168100.000000.830560.001340.83190H430.196380.000000.802010.001610.80362H440.200120.000000.798210.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.800090.001490.80158H470.180190.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999484.325010.013626.33811	С	41	-0.33321	1.99951	4.32024	0.01346	6.33321			
H430.196380.000000.802010.001610.80362H440.200120.000000.798210.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.800090.001490.80158H470.180190.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999484.325010.013626.33811	Н	42	0.16810	0.00000	0.83056	0.00134	0.83190			
H440.200120.000000.798210.001660.79988C45-0.170041.999384.153700.016966.17004H460.198420.000000.800090.001490.80158H470.180190.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999484.325010.013626.33811	H	43	0.19638	0.00000	0.80201	0.00161	0.80362			
C 45 -0.17004 1.99938 4.15370 0.01696 6.17004 H 46 0.19842 0.00000 0.80009 0.00149 0.80158 H 47 0.18019 0.00000 0.81835 0.00146 0.81981 C 48 -0.16927 1.99939 4.15317 0.01671 6.16927 H 49 0.19278 0.00000 0.80571 0.00151 0.80722 H 50 0.18380 0.00000 0.81471 0.00149 0.81620 N 51 -0.65432 1.99961 5.62975 0.02496 7.65432 C 52 -0.33811 1.99948 4.32501 0.01362 6.33811	H	44	0.20012	0.00000	0.79821	0.00166	0.79988			
H460.198420.000000.800090.001490.80158H470.180190.000000.818350.001460.81981C48-0.169271.999394.153170.016716.16927H490.192780.000000.805710.001510.80722H500.183800.000000.814710.001490.81620N51-0.654321.999615.629750.024967.65432C52-0.338111.999484.325010.013626.33811	C	45	-0.17004	1.99938	4.15370	0.01696	6.17004			
H 47 0.18019 0.00000 0.81835 0.00146 0.81981 C 48 -0.16927 1.99939 4.15317 0.01671 6.16927 H 49 0.19278 0.00000 0.80571 0.00151 0.80722 H 50 0.18380 0.00000 0.81471 0.00149 0.81620 N 51 -0.65432 1.99961 5.62975 0.02496 7.65432 C 52 -0.33811 1.99948 4.32501 0.01362 6.33811	H 	46	0.19842	0.00000	0.80009	0.00149	0.80158			
C 48 -0.16927 1.99939 4.15317 0.01671 6.16927 H 49 0.19278 0.00000 0.80571 0.00151 0.80722 H 50 0.18380 0.00000 0.81471 0.00149 0.81620 N 51 -0.65432 1.99961 5.62975 0.02496 7.65432 C 52 -0.33811 1.99948 4.32501 0.01362 6.33811	H	47	0.18019	0.00000	0.81835	0.00146	0.81981			
H 49 0.19278 0.00000 0.80571 0.00151 0.80722 H 50 0.18380 0.00000 0.81471 0.00149 0.81620 N 51 -0.65432 1.99961 5.62975 0.02496 7.65432 C 52 -0.33811 1.99948 4.32501 0.01362 6.33811	C.	48	-0.1027	T.99939	4.15317	U.U1671	6.16927			
R 50 0.18380 0.00000 0.81471 0.00149 0.81620 N 51 -0.65432 1.99961 5.62975 0.02496 7.65432 C 52 -0.33811 1.99948 4.32501 0.01362 6.33811	H	49 50	U.192/8 0 10200	0.00000	0.005/L	0.00140	0.80/22			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	п м	50	U. 1030U	1 00000	U.014/1 5 62075	0.00149	U.0102U 7 65422			
	л Г	52 52	-0.33811	1,99948	4.32501	0.02490	6 33811			

	Н Н Н С Н С Н С Н С Н С	53 54 55 56 57 58 59 60 61 62 63 64 65	0.16705 0.22421 0.18694 -0.33462 0.18673 0.21893 0.16574 0.01895 -0.56242 0.18940 -0.28716 0.18130 -0.30196	0.00000 0.00000 1.99949 0.00000 0.00000 1.99909 1.99926 0.00000 1.99931 0.00000 1.99932	0.831 0.774 0.811 4.321 0.812 0.779 0.832 3.953 4.522 0.808 4.255 0.816 4.269	.56 0 .08 0 .67 0 .66 0 .02 0 .95 0 .95 0 .74 0 .42 0 .93 0	.00139 .00171 .00139 .01348 .00125 .00180 .00131 .02801 .04078 .00186 .03244 .00177 .03278	0.83295 0.77579 0.81306 6.33462 0.81327 0.78107 0.83426 5.98105 6.56242 0.81060 6.28716 0.81870 6.30196
	H C	66 67	-0.54347	0.00000 1.99925	0.815 4.505	48 0 76 0	.00175 .03847	0.81722 6.54347
=	H ======	68 ====	0.18806	0.00000	0.810	02 0	.00192 =======	0.81194
	* Tota	1 *	0.00000	55.98277	149.278	73 0	.73851 2	206.00000
_				Natur	al Popul	ation		
_	Core Valenc Natura Natura	e l Mir l Ryc	nimal Basis Aberg Basis	55.98277 149.27873 205.26149 0.73851	(99.969 (99.519 (99.641 (0.358	2% of 2% of 1 5% of 2 5% of 2	56) 50) 06) 06)	
_	Atom	No	Natura	al Electron	n Configu	ration		
	Ы	1 2	[core]2S((0.08)30(0)	20)2d((0.01)	(0,02)	
	C	∠ 3	[core]2S(1.32/2p(4)	32)3d(0.01)4p	(0.02)	
	H	4	1S(0.80)		0.01/12	(0.01)	
	Н	5	1S (0.81)				
	Н	6	1S (0.83)				
	С	7	[core]2S(1.01)2p(3	.31)3d(0.01)4p	(0.01)	
	Н	8	1S(0.83)				
	H	9	1S(0.80)				
	H	10	ls((0.80)	10)27(0 01 \ 4-	(0 01)	
	U U	12	[core]25(0.97)2p(3	.18)30(0.01)4p	(0.01)	
	н Н	13	15(0.82)				
	C	14	[core]2S(0.97)2p(3	.18)3d(0.01)4p	(0.01)	
	Н	15	1S (0.81)				
	Н	16	1S(0.81)				
	N	17	[core]2S(1.32)2p(4	.31)3d(0.01)4p	(0.01)	
	C	18	[core]2S(1.01)2p(3	.31)3d(0.01)4p	(0.01)	
	H	19	1S(0.83)				
	H	20	IS (0.77)				
	н С	∠⊥ 22	LS ((0.81)	21)27(0 01)40	(0 01)	
	с н	22	[COLE]25(15(0 81)	0.51/5u(0.01/40	(0.01)	
	H	2.4	15(0.78)				
	H	25	1S (0.83)				
	С	26	[core]2S(0.88)2p(3	.07)3p(0.01)3d	(0.01)4p	(0.01)
	С	27	[core]2S(0.92)2p(3	.61)4p(0.03)	-	
	Н	28	1S (0.81)				
	С	29	[core]2S(0.93)2p(3	.33)4p(0.02)		
	ц	30	15(0 82)				
	11			0.02)	- · · · ·			

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Н	32	1S (0.82)				
С	33	[core]2S(0.91)2p(3.59)4p(0.03)		
Н	34	1S (0.81)	_			
Li	35	[core]2S(0.08)3d(0.01)4p(0.01)		
Ν	36	[core]2S(1.32)2p(4.30)3d(0.01)4p(0.02)	
С	37	[core]2S(1.01)2p(3.32)3d(0.01)4p(0.01)	
Η	38	1S (0.80)				
Η	39	1S (0.81)				
Η	40	1S (0.83)				
С	41	[core]2S(1.01)2p(3.31)3d(0.01)4p(0.01)	
Η	42	1S (0.83)				
Η	43	1S (0.80)				
Η	44	1S (0.80)				
С	45	[core]2S(0.97)2p(3.18)3d(0.01)4p(0.01)	
Η	46	1S (0.80)				
Η	47	1S (0.82)				
С	48	[core]2S(0.97)2p(3.18)3d(0.01)4p(0.01)	
Η	49	1S (0.81)				
Η	50	1S (0.81)				
Ν	51	[core]2S(1.32)2p(4.31)3d(0.01)4p(0.01)	
С	52	[core]2S(1.01)2p(3.31)3d(0.01)4p(0.01)	
Η	53	1S (0.83)				
Η	54	1S (0.77)				
Η	55	1S (0.81)				
С	56	[core]2S(1.01)2p(3.31)3d(0.01)4p(0.01)	
Η	57	1S (0.81)				
Η	58	1S (0.78)				
Η	59	1S (0.83)				
С	60	[core]2S(0.88)2p(3.07)3p(0.01)3d(0.01)4p(0.01)
С	61	[core]2S(0.92)2p(3.61)4p(0.03)		
Η	62	1S (0.81)				
С	63	[core]2S(0.93)2p(3.33)4p(0.02)		
Η	64	1S (0.82)				
С	65	[core]2S(0.93)2p(3.34)4p(0.02)		
Η	66	1S(0.82)				
С	67	[core]2S(0.91)2p(3.59)4p(0.03)		
Η	68	1S (0.81)				

NBO analysis skipped by request.

1|1|UNPC-UNK|SP|RHF|6-31+G(d,p)|C22H40Li2N4|PCUSER|02-Sep-2008|0||# HF /6-31+G(D,P) POP=(NPA,FULL) GEOM=CONNECTIVITY SCF=TIGHT INT=ULTRAFINE Single point on 2 | 0,1 Li N,1,2.12275239 C,2,1.45922543,1,106.58359 672 | H, 3, 0.95993404, 2, 109.47987106, 1, 68.7306377, 0 | H, 3, 0.95978992, 2, 109. 45930829,1,-51.24126721,0 H,3,0.95990392,2,109.46293755,1,-171.2879933 ,0|C,2,1.45677212,1,116.24538622,3,122.11570946,0|H,7,0.95997646,2,109 .50539566,1,178.57829491,0 H,7,0.9598592,2,109.5146923,1,58.50375648,0 |H,7,0.96069526,2,109.47933752,1,-61.46509045,0|C,2,1.46889305,1,103.8 4294701,3,-117.11645077,0 H,11,0.97023252,2,109.20467954,1,-79.4609245 1,0|H,11,0.96968767,2,109.20598111,1,162.69895523,0|C,11,1.50920707,2, 111.99365366,1,41.60879241,0 | H,14,0.96990107,11,109.37569001,2,66.3139 3929,0 | H,14,0.96955258,11,109.33417399,2,-175.61174162,0 | N,14,1.463974 51,11,111.31579847,2,-54.66721341,0 C,17,1.46333286,14,110.91788568,11 ,-78.12473783,0|H,18,0.95972205,17,109.47692249,14,-59.50667739,0|H,18 ,0.95978967,17,109.48126841,14,-179.5447939,0|H,18,0.96033041,17,109.4 8165817,14,60.4845624,0 C,17,1.46103898,14,110.03736109,11,160.7376311 8,0|H,22,0.96023482,17,109.50323596,14,-59.76055302,0|H,22,0.96017707, 17,109.43923217,14,-179.75373608,0 | H,22,0.96006393,17,109.48198252,14, 60.24861259,0 | C,1,2.61216876,2,145.37721711,7,-28.28319714,0 | C,26,1.42 140755,1,61.8640062,2,45.90731574,0 | H,27,0.93007073,26,119.39920175,1, -115.26555427,0 | C,27,1.43412045,26,121.23681398,1,64.76636099,0 | H,29,0

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.93047313,27,120.21929297,26,164.8650778,0/C,29,1.36283671,27,119.5255 9339,26,-15.13703593,0|H,31,0.92983066,29,120.37102273,27,-179.0110921 1,0 | C,31,1.43624804,29,119.32314263,27,0.97132326,0 | H,33,0.92987985,31 ,119.29773231,29,-166.29894867,0|Li,26,2.60977624,1,147.63983696,2,-17 9.47269208,0 N,35,2.12275239,26,177.71876604,1,-7.54852098,0 C,36,1.45 922543,35,106.58359672,26,157.50758299,0|H,37,0.95993404,36,109.479871 06,35,-68.7306377,0|H,37,0.95978992,36,109.45930829,35,51.24126721,0|H ,37,0.95990392,36,109.46293755,35,171.2879933,0 C,36,1.45677212,35,116 .24538622,26,35.39187353,0 H,41,0.95997646,36,109.50539566,35,-178.578 29491,0 | H,41,0.9598592,36,109.5146923,35,-58.50375648,0 | H,41,0.9606952 6,36,109.47933752,35,61.46509045,0 C,36,1.46889305,35,103.84294701,26, -85.37596623,0|H,45,0.97023252,36,109.20467954,35,79.46092451,0|H,45,0 .96968767,36,109.20598111,35,-162.69895523,0|C,45,1.50920707,36,111.99 365366,35,-41.60879241,0|H,48,0.96990107,45,109.37569001,36,-66.313939 29,0|H,48,0.96955258,45,109.33417399,36,175.61174162,0|N,48,1.46397451 ,45,111.31579847,36,54.66721341,0 C,51,1.46333286,48,110.91788568,45,7 8.12473783,0|H,52,0.95972205,51,109.47692249,48,59.50667739,0|H,52,0.9 5978967,51,109.48126841,48,179.5447939,0 | H,52,0.96033041,51,109.481658 17,48,-60.4845624,0 C,51,1.46103898,48,110.03736109,45,-160.73763118,0 |H,56,0.96023482,51,109.50323596,48,59.76055302,0|H,56,0.96017707,51,1 09.43923217,48,179.75373608,0 H,56,0.96006393,51,109.48198252,48,-60.2 4861259,0 C,33,1.41420858,31,121.45757832,29,13.7272786,0 C,60,1.42140 755,33,124.60868346,31,166.05739581,0 | H,61,0.93007073,60,119.39920175, 33,-14.40723538,0 | C,61,1.43412045,60,121.23681398,33,165.56084937,0 | H, 63,0.93047313,61,120.21929297,60,-164.8650778,0|C,63,1.36283671,61,119 .52559339,60,15.13703593,0 H,65,0.92983066,63,120.37102273,61,179.0110 9211,0 C,26,1.41420858,1,136.98552198,2,-65.86852632,0 H,67,0.92987985 ,26,119.24468425,1,98.16379666,0 || Version=IA32L-G03RevC.02 |State=1 -AG|HF=-1088.5310227|RMSD=5.937e-009|Dipole=0.,0.,0.|PG=CI [X(C22H40Li 2N4)]||@

2.3. HF/6-311++G(d,p)

		Noturol	Natural Population				
Atom	No	Charge	Core	Valence	Rydberg	Total	
Li	1	0.85899	1.99923	0.11352	0.02826	2.14101	
Ν	2	-0.62061	1.99961	5.59465	0.02635	7.62061	
С	3	-0.22488	1.99914	4.21235	0.01339	6.22488	
Н	4	0.15934	0.00000	0.83860	0.00207	0.84066	
Н	5	0.14843	0.00000	0.84997	0.00160	0.85157	
Н	6	0.13026	0.00000	0.86793	0.00181	0.86974	
С	7	-0.21550	1.99913	4.20348	0.01288	6.21550	
Н	8	0.12717	0.00000	0.87112	0.00171	0.87283	
Н	9	0.15348	0.00000	0.84495	0.00157	0.84652	
Н	10	0.15711	0.00000	0.84127	0.00162	0.84289	
С	11	-0.07133	1.99905	4.05581	0.01647	6.07133	
Н	12	0.14759	0.00000	0.85060	0.00182	0.85241	
Н	13	0.13136	0.00000	0.86659	0.00205	0.86864	
С	14	-0.07163	1.99906	4.05637	0.01620	6.07163	
H	15	0.14255	0.00000	0.85567	0.00179	0.85745	
Н	16	0.13562	0.00000	0.86241	0.00197	0.86438	
Ν	17	-0.62449	1.99961	5.60186	0.02302	7.62449	
С	18	-0.22693	1.99911	4.20784	0.01998	6.22693	
Н	19	0.12689	0.00000	0.87170	0.00141	0.87311	

Н	20	0.18445	0.00000	0.81378	0.00177	0.81555
Н	21	0.14587	0.00000	0.85280	0.00133	0.85413
C	22	-0.21810	1.99912	4.20614	0.01285	6.21810
H	23	0.14395	0.00000	0.85472	0.00133	0.85605
Н	24	0.17783	0.00000	0.82058	0.00159	0.82217
Н	25	0.12484	0.00000	0.87354	0.00162	0.87516
C	26	0.01647	1.99918	3.95496	0.02939	5.98353
C	27	-0.52283	1.99917	4.48386	0.03980	6.52283
H	28	0.15002	0.0000	0.84760	0.00238	0.84998
С	29	-0.24112	1.99929	4.21219	0.02964	6.24112
Н	30	0.14081	0.00000	0.85722	0.00197	0.85919
C	31	-0.25630	1.99929	4.22593	0.03109	6.25630
Н	32	0.14273	0.00000	0.85537	0.00190	0.85727
С	33	-0.50990	1.99916	4.46739	0.04334	6.50990
H	34	0.14929	0.00000	0.84841	0.00230	0.85071
Li	35	0.85762	1.99923	0.11351	0.02964	2.14238
N	36	-0.62074	1.99961	5.59463	0.02650	7.62074
C	37	-0.22490	1.99914	4.21237	0.01340	6.22490
H	38	0.15933	0.0000	0.83860	0.00207	0.84067
H	39	0.14843	0.0000	0.84998	0.00160	0.85157
H	40	0.13026	0.0000	0.86793	0.00181	0.86974
C	41	-0.21550	1.99913	4.20348	0.01288	6.21550
H	42	0.12718	0.0000	0.87112	0.00171	0.87282
H	43	0.15347	0.0000	0.84495	0.00157	0.84653
H	44	0.15711	0.0000	0.84127	0.00163	0.84289
C	45	-0.07133	1.99905	4.05580	0.01648	6.07133
Н	46	0.14758	0.00000	0.85060	0.00182	0.85242
Н	47	0.13136	0.00000	0.86659	0.00205	0.86864
C	48	-0.07164	1.99906	4.05637	0.01621	6.07164
Н	49	0.14255	0.00000	0.85567	0.00179	0.85745
Н	50	0.13562	0.00000	0.86241	0.00197	0.86438
N	51	-0.62453	1.99961	5.60189	0.02303	7.62453
C	52	-0.22696	1.99911	4.20783	0.02001	6.22696
Н	53	0.12689	0.00000	0.87170	0.00141	0.87311
H	54	0.18443	0.0000	0.81377	0.00180	0.81557
Н	55	0.14587	0.00000	0.85281	0.00133	0.85413
C	56	-0.21811	1.99912	4.20614	0.01285	6.21811
Н	57	0.14395	0.00000	0.85472	0.00133	0.85605
Н	58	0.17782	0.00000	0.82058	0.00160	0.82218
Н	59	0.12484	0.00000	0.87354	0.00162	0.87516
C	60	0.02464	1.99917	3.94698	0.02922	5.97536
C	61	-0.52259	1.99917	4.48370	0.03973	6.52259
Н	62	0.14998	0.00000	0.84763	0.00239	0.85002
C	63	-0.24101	1.99929	4.21222	0.02949	6.24101
Н	64	0.14079	0.00000	0.85722	0.00199	0.85921
C	65	-0.26095	1.99931	4.23014	0.03150	6.26095
Н	66	0.14271	0.00000	0.85535	0.00194	0.85729
C	67	-0.49309	1.99889	4.45066	0.04354	6.49309
H	68	0.14753	0.00000	0.84996	0.00251	0.85247
* Tota	===== 1 *	0.00000	55.97805	149.26328	0.75867	206.00000
			Natur	cal Populatio	n	
Core			55.97805	(99.9608% 0	f 56)	
Valenc	ce		149.26328	(99.5089% o	f 150)	
Natura	al Min	nimal Basis	205.24133	(99.6317% 0	£ 206)	
Natura	al Ryo	dberg Basis	0.75867	(0.3683% 0	f 206)	

Atom No Natural Electron Configuration

T.i	1	[core]29(0.11)3d(0.01)4n(0.01)
м	1	$\begin{bmatrix} core \end{bmatrix} 23 \begin{pmatrix} core \\ core \\ core \end{bmatrix} 23 \begin{pmatrix} core \\ core \\ core \end{bmatrix} 23 \begin{pmatrix} core \\ core \\ core \\ core \end{bmatrix} 23 \begin{pmatrix} core \\ $	1 - 22 + 2n(4 - 27) + 2n(-0 - 01) + n(-0 - 01)
N	2	[COIE] 25 (1.32/2p(4.27)3p(0.01)4p(0.01)
	3	[core]2S(0.96)2p(3.25)3d(0.01)
Н	4	1S (0.84)
Н	5	1S (0.85)
Н	6	1S(0.87)
С	7	[core]2S(0.96)2p(3.25)3d(0.01)
Н	8	1S (0.87)
Н	9	1S(0.84)
Н	10	1S (0.84)
С	11	[core]2S(0.94)2p(3.12)3p(0.01)3d(0.01)
Н	12	1S(0.85)
Н	13	1S(0.87)
С	14	[core]2S(0.93)2p(3.12)3p(0.01)3d(0.01)
Н	15	1S (0.86)
Н	16	1S (0.86)
N	17	[core]2S(1 32)2n(4 28)4n(0 01)
C	18	[core]25(0.96)2n(3.25)3d(0.01)
ч Ч	19	19(0.87)
и и	20	19(0.81)
11 11	20	10(
п	21		0.00)
	22	[COTE]25(0.96)2p(3.25)3d(0.01)
H	23	15(0.85)
H	24	1S (0.82)
H	25	IS ((0.87)
C	26	[core]2S(0.88)2p(3.08)3d(0.01)4p(0.02)
C	27	[core]2S((0.89)2p(3.59)4p(0.03)
Н	28	1S (0.85)
C	29	[core]2S(0.90)2p(3.31)3d(0.01)4p(0.02)
Н	30	1S (0.86)
С	31	[core]2S(0.90)2p(3.32)3d(0.01)4p(0.02)
Н	32	1S(0.86)
C	33	[core]2S(0.89)2p(3.58)3p(0.01)4p(0.03)
Н	34	1S(0.85)
Li	35	[core]2S(0.11)3d(0.01)4p(0.02)
N	36	[core]2S(1.32)2p(4.27)3p(0.01)4p(0.01)
С	37	[core]2S(0.96)2p(3.25)3d(0.01)
Н	38	1S(0.84)
Н	39	1S(0.85)
Н	40	1S(0.87)
С	41	[core]2S(0.96)2p(3.25)3d(0.01)
Н	42	1S(0.87)
Н	43	1S(0.84)
Н	44	1S(0.84)
С	45	[core]2S(0.94)2p(3.12)3p(0.01)3d(0.01)
Н	46	1S(0.85)
Н	47	1S (0.87)
С	48	[core]2S($(0.93)_{2p}(3.12)_{3p}(0.01)_{3d}(0.01)$
Н	49	1S(0.86)
н	50	15(0.86)
N	51	[corel25(1.32)2p(4.28)4p(0.01)
C	52	[core]29(0.96)2p(3.25)3d(0.01)
н Н	53	19/	0.87)
и Ц	54	1C/	0.81)
ч		10(10 <i>(</i>	0.85)
C	56	Lo ([corel 20 (0.00, 0.96)2n(3.25)3d(0.01)
с ц	57	10/	0.85)
и П	58	10(10/	0.82)
л u	50	10(10(0.02/
11		TD (0.077

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С	60	[core]2S(0.87)2p(3.07)3d(0.01)4p(0.02)	
С	61	[core]2S(0.89)2p(3.59)4p(0.03)		
Η	62	1S (0.85)				
С	63	[core]2S(0.90)2p(3.31)3p(0.01)3d(0.01)4p(0.01)
Н	64	1S (0.86)				
С	65	[core]2S(0.91)2p(3.32)4p(0.02)		
Η	66	1S (0.86)				
С	67	[core]2S(0.87)2p(3.58)3p(0.01)4p(0.03)	
Н	68	1S (0.85)				

NBO analysis skipped by request.

1|1|UNPC-UNK|SP|RHF|6-311++G(d,p)|C22H40Li2N4|PCUSER|06-Sep-2008|0||# HF/6-311++G(D,P) POP=(NPA,FULL) GEOM=CONNECTIVITY INT=ULTRAFINE SCF=TI GHT||Single point on 2||0,1|Li|N,1,2.12275239|C,2,1.45922543,1,106.5 8359672 H, 3, 0.95993404, 2, 109.47987106, 1, 68.7306377, 0 H, 3, 0.95978992, 2, 109.45930829,1,-51.24126721,0|H,3,0.95990392,2,109.46293755,1,-171.287 9933,0 C,2,1.45677212,1,116.24538622,3,122.11570946,0 H,7,0.95997646,2 ,109.50539566,1,178.57829491,0 | H,7,0.9598592,2,109.5146923,1,58.503756 48,0 | H,7,0.96069526,2,109.47933752,1,-61.46509045,0 | C,2,1.46889305,1,1 03.84294701,3,-117.11645077,0|H,11,0.97023252,2,109.20467954,1,-79.460 92451,0|H,11,0.96968767,2,109.20598111,1,162.69895523,0|C,11,1.5092070 7,2,111.99365366,1,41.60879241,0|H,14,0.96990107,11,109.37569001,2,66. 31393929,0 | H,14,0.96955258,11,109.33417399,2,-175.61174162,0 | N,14,1.46 397451,11,111.31579847,2,-54.66721341,0|C,17,1.46333286,14,110.9178856 8,11,-78.12473783,0|H,18,0.95972205,17,109.47692249,14,-59.50667739,0| H,18,0.95978967,17,109.48126841,14,-179.5447939,0|H,18,0.96033041,17,1 09.48165817,14,60.4845624,0 | C,17,1.46103898,14,110.03736109,11,160.737 63118,0 | H, 22,0.96023482,17,109.50323596,14,-59.76055302,0 | H, 22,0.96017 707,17,109.43923217,14,-179.75373608,0|H,22,0.96006393,17,109.48198252 ,14,60.24861259,0|C,1,2.61216876,2,145.37721711,7,-28.28319714,0|C,26, 1.42140755,1,61.8640062,2,45.90731574,0|H,27,0.93007073,26,119.3992017 5,1,-115.26555427,0|C,27,1.43412045,26,121.23681398,1,64.76636099,0|H, 29,0.93047313,27,120.21929297,26,164.8650778,0 C,29,1.36283671,27,119. 52559339,26,-15.13703593,0|H,31,0.92983066,29,120.37102273,27,-179.011 09211,0 C,31,1.43624804,29,119.32314263,27,0.97132326,0 H,33,0.9298798 5,31,119.29773231,29,-166.29894867,0 Li,26,2.60977624,1,147.63983696,2 ,-179.47269208,0 N,35,2.12275239,26,177.71876604,1,-7.54852098,0 C,36, 1.45922543,35,106.58359672,26,157.50758299,0 | H,37,0.95993404,36,109.47 987106,35,-68.7306377,0|H,37,0.95978992,36,109.45930829,35,51.24126721 ,0|H,37,0.95990392,36,109.46293755,35,171.2879933,0|C,36,1.45677212,35 ,116.24538622,26,35.39187353,0 | H,41,0.95997646,36,109.50539566,35,-178 .57829491,0|H,41,0.9598592,36,109.5146923,35,-58.50375648,0|H,41,0.960 69526,36,109.47933752,35,61.46509045,0 C,36,1.46889305,35,103.84294701 ,26,-85.37596623,0|H,45,0.97023252,36,109.20467954,35,79.46092451,0|H, 45,0.96968767,36,109.20598111,35,-162.69895523,0 C,45,1.50920707,36,11 1.99365366,35,-41.60879241,0 | H,48,0.96990107,45,109.37569001,36,-66.31 393929,0 | H,48,0.96955258,45,109.33417399,36,175.61174162,0 | N,48,1.4639 7451,45,111.31579847,36,54.66721341,0 C,51,1.46333286,48,110.91788568, 45,78.12473783,0 | H,52,0.95972205,51,109.47692249,48,59.50667739,0 | H,52 ,0.95978967,51,109.48126841,48,179.5447939,0 H,52,0.96033041,51,109.48 165817,48,-60.4845624,0 | C,51,1.46103898,48,110.03736109,45,-160.737631 18,0 | H,56,0.96023482,51,109.50323596,48,59.76055302,0 | H,56,0.96017707, 51,109.43923217,48,179.75373608,0 H,56,0.96006393,51,109.48198252,48,-60.24861259,0 | C,33,1.41420858,31,121.45757832,29,13.7272786,0 | C,60,1.4 2140755,33,124.60868346,31,166.05739581,0|H,61,0.93007073,60,119.39920 175,33,-14.40723538,0 C,61,1.43412045,60,121.23681398,33,165.56084937, 0 | H, 63, 0.93047313, 61, 120.21929297, 60, -164.8650778, 0 | C, 63, 1.36283671, 61 ,119.52559339,60,15.13703593,0 H,65,0.92983066,63,120.37102273,61,179. 01109211,0 | C,26,1.41420858,1,136.98552198,2,-65.86852632,0 | H,67,0.9298 7985,26,119.24468425,1,98.16379666,0|| Version=IA32L-G03RevC.02|Sta

te=1-AG|HF=-1088.7246449|RMSD=6.864e-009|Dipole=0.,0.,0.|PG=CI [X(C22H 40Li2N4)]|@

2.4. B3LYP/6-31+G(d,p)

		Noture 1		Natural Pop	ulation	
 Atom	No	Charge	Core	Valence	Rydberg	Total
Li	1	0.87925	1.99891	0.09228	0.02956	2.12075
Ν	2	-0.59184	1.99961	5.56753	0.02471	7.59184
С	3	-0.41882	1.99945	4.40801	0.01136	6.41882
Н	4	0.22133	0.00000	0.77612	0.00255	0.77867
Н	5	0.21064	0.00000	0.78806	0.00130	0.78936
Н	6	0.18961	0.00000	0.80852	0.00187	0.81039
С	7	-0.41173	1.99946	4.40168	0.01059	6.41173
Н	8	0.18691	0.00000	0.81140	0.00169	0.81309
Н	9	0.21650	0.00000	0.78186	0.00164	0.78350
Н	10	0.22031	0.00000	0.77782	0.00187	0.77969
С	11	-0.22867	1.99933	4.21575	0.01360	6.22867
Н	12	0.21862	0.00000	0.77994	0.00144	0.78138
Н	13	0.20033	0.00000	0.79758	0.00209	0.79967
С	14	-0.22791	1.99934	4.21522	0.01335	6.22791
Н	15	0.21333	0.00000	0.78525	0.00142	0.78667
Н	16	0.20375	0.00000	0.79407	0.00218	0.79625
Ν	17	-0.59555	1.99960	5.57287	0.02307	7.59555
С	18	-0.41748	1.99943	4.40694	0.01111	6.41748
Н	19	0.18651	0.00000	0.81164	0.00185	0.81349
Н	20	0.24305	0.00000	0.75541	0.00154	0.75695
Н	21	0.20759	0.00000	0.79115	0.00126	0.79241
С	22	-0.41349	1.99944	4.40327	0.01078	6.41349
Н	23	0.20802	0.00000	0.79083	0.00115	0.79198
Н	24	0.23651	0.00000	0.76145	0.00204	0.76349
Н	25	0.18537	0.00000	0.81297	0.00165	0.81463
С	26	-0.04647	1.99910	4.02440	0.02298	6.04647
С	27	-0.51252	1.99924	4.48124	0.03204	6.51252
Н	28	0.19727	0.00000	0.80055	0.00219	0.80273
С	29	-0.32180	1.99930	4.29604	0.02645	6.32180
Н	30	0.19389	0.00000	0.80415	0.00197	0.80611
С	31	-0.33226	1.99931	4.30644	0.02651	6.33226
Η	32	0.19529	0.00000	0.80278	0.00193	0.80471
С	33	-0.49354	1.99923	4.46504	0.02926	6.49354
H	34	0.19611	0.00000	0.80162	0.00227	0.80389
Li	35	0.87868	1.99891	0.09219	0.03022	2.12132
Ν	36	-0.59203	1.99961	5.56754	0.02488	7.59203
С	37	-0.41898	1.99945	4.40802	0.01151	6.41898
Н	38	0.22109	0.00000	0.77611	0.00280	0.77891
Н	39	0.21063	0.00000	0.78806	0.00130	0.78937
H	40	0.18960	0.00000	0.80852	0.00188	0.81040
С	41	-0.41192	1.99946	4.40169	0.01077	6.41192
Н	42	0.18691	0.00000	0.81140	0.00169	0.81309
Н	43	0.21645	0.00000	0.78186	0.00169	0.78355
Н	44	0.22033	0.00000	0.77785	0.00183	0.77967
C	45	-0.22875	1.99933	4.21574	0.01368	6.22875
H	46	0.21863	0.00000	0.77994	0.00144	0.78137

	НСННИСНННССНС	47 48 49 50 51 52 53 54 55 57 58 59 60 61 62 63	0.20033 - 0.22788 0.21334 0.20375 - 0.59565 - 0.41732 0.18652 0.24309 0.20759 - 0.41347 0.20802 0.23663 0.18538 - 0.04688 - 0.54599 0.19673 - 0.20676	0.00000 1.99934 0.00000 1.99960 1.99943 0.00000 0.00000 0.00000 1.99944 0.00000 0.00000 1.99944 0.00000 1.99910 1.99930 0.00000 1.99932	0.79757 4.21522 0.78524 0.79407 5.57290 4.40687 0.81164 0.75539 0.79115 4.40326 0.79083 0.76146 0.81298 4.02500 4.49961 0.80063 4.19117	0.00210 0.01332 0.00142 0.00218 0.02315 0.01102 0.00184 0.00151 0.00126 0.01077 0.00114 0.00191 0.00164 0.02278 0.04708 0.00264 0.01627	0.79967 6.22788 0.78666 0.79625 7.59565 6.41732 0.81348 0.75691 0.79241 6.41347 0.79198 0.76337 0.81462 6.04688 6.54599 0.80327 6.20676	
	Н	64	0.17484	0.00000	0.82030	0.00486	0.82516	
	C	65	-0.37073	1.99939	4.33025	0.04109	6.37073	
	н	66	0.19487	0.00000	0.80282	0.00232	0.80513	
	С Н	67 68	-0.49270	1.99923	4.46514	0.02834 0.00240	6.49270 0.80394	
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*	* Tota	1 *	0.01850	55.98166	149.33387	0.66597	205.98150	
				Natur	al Population	l		
כ ע וו וו	Core Valenc Natura Natura	e 1 Mi: 1 Ry	nimal Basis dberg Basis	55.98166 149.33387 205.31553 0.66597	(99.9673% of (99.5559% of (99.6677% of (0.3233% of	E 56) E 150) E 206) E 206)		
	Atom	No	Natura	al Electron	Configuratio	on		-
	Atom 	No 	Natura	al Electron	Configuratio	on 		-
	Atom Li	No 1	Natura [core]2S(al Electron 0.09)3d(0	Configuratio	n 		-
	Atom Li N	No 1 2	Natura [core]2S([core]2S(al Electron 0.09)3d(0 1.31)2p(4	.01)4p(0.01)	n 		-
	Atom Li N C	No 1 2 3	Natur; [core]2S([core]2S([core]2S(al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3	Configuratio	on))		-
	Atom Li N C H	No 1 2 3 4	Natur; [core]2S([core]2S([core]2S(1S(al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78)	Configuratio	on))		-
	Atom Li N C H H	No 1 2 3 4 5 6	Natur; [core]2S([core]2S([core]2S(1S(1S(al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81)	Configuratio	on))		-
	Atom Li N C H H H C	No 1 2 3 4 5 6 7	Natur; [core]2S([core]2S([core]2S(1S(1S(1S(1S(al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3	Configuratio	on 		-
	Atom Li N C H H H C H	No 1 2 3 4 5 6 7 8	Natur: [core]2S([core]2S([core]2S(1S(1S(1S([core]2S(1S(al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81)	Configuratio	on)))		-
	Atom Li N C H H H C H H H H	No 2 3 4 5 6 7 8 9	Natura [core]2S([core]2S([core]2S(1S(1S(1S([core]2S(1S(1S(1S(al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 0.81) 0.78)	Configuratio	on)))		-
	Atom Li N C H H H C H H H H	No 1 2 3 4 5 6 7 8 9 10	Natura [core]2S([core]2S([core]2S(1S(1S([core]2S(1S(1S(1S(1S(1S(1S(al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 0.81) 0.78) 0.78)	Configuratio	on 		-
	Atom Li N C H H H C H H C H H C	No 1 2 3 4 5 6 7 8 9 10 11	Natur; [core]2S([core]2S([core]2S(1S(1S([core]2S(1S(1S(1S(1S(1S(2S(al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78)	Configuratio	on)))		_
	Atom Li N C H H H C H H C H H H C H	No 1 2 3 4 5 6 7 8 9 10 11 12	Natur; [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78)	Configuratio	on)))		-
	Atom Li N C H H H C H H C H H C H H C H H C	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14	Natura [core]2S([core]2S([core]2S(1S(1S(1S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 0.78] 0.78] 0	Configuratio	on 		-
	Atom Li N C H H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H C H H C H N C H C H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	Natura [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.97)2p(3 0.97)2p(3 0.97)2p(3 0.97)2p(3)	Configuratio .01)4p(0.01) .25)4p(0.01) .40)4p(0.01) .39)4p(0.01) .24)4p(0.01)	on 		-
	Atom Li N C H H H C H H C H H C H H C H H C H H C H H C H H H C H H H C H H H C H H H H C H H H H C H H H H C H H H H H C H H H H H C H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	Natura [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 1.01)2p(3 0.81) 0.78) 0.78) 0.78) 0.78) 0.97)2p(3 0.79) 0.80) 0.97)2p(3 0.79) 0.79)	Configuratio	on)))		_
	Atom Li N C H H C H H C H H C H H C H H N C H H N C H H H N C H H H N C H H H N C H H H N C H H H H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	Natura [core] 2S ([core] 2S ([core] 2S (1S (1S (1S (1S (1S (1S (1S (1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 1.01)2p(3 0.81) 0.78) 0.78) 0.78) 0.78) 0.97)2p(3 0.79) 0.80) 0.97)2p(3 0.79) 0.79) 0.79) 1.32)2p(4	Configuratio	on)))		_
	Atom Li N C H H C H H C H H C H H C H H N C H H C H H C H H C H H C H H C H H C H H C H H C H C H H C H N C H C H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	Natur: [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 1.01)2p(3 0.78) 0.78) 0.97)2p(3 0.78) 0.97)2p(3 0.79) 0.80) 0.97)2p(3 0.79) 0.79) 1.32)2p(4 1.01)2p(3	Configuratio .01)4p(0.01) .25)4p(0.01) .40)4p(0.01) .39)4p(0.01) .24)4p(0.01) .24)4p(0.01) .24)4p(0.01) .26)4p(0.01) .39)4p(0.01)	on))))		
	Atom Li N C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H C H H H C H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H H C H H H H C H H H H C H H H H C H H H H C H H H H C H H H H H C H H H H H C H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	Natura [core] 2S ([core] 2S ([core] 2S (1S (1S (1S (1S (1S (1S (1S (1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.97)2p(3 0.79) 0.79) 0.79) 1.32)2p(4 1.01)2p(3 0.81)	Configuratio .01)4p(0.01) .25)4p(0.01) .40)4p(0.01) .39)4p(0.01) .24)4p(0.01) .24)4p(0.01) .24)4p(0.01) .26)4p(0.01) .39)4p(0.01)	on))))		
	Atom Li N C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H H C H H H H C H H H H C H H H H H C H H H H H C H H H H H C H H H H C H H H H H C H H H H H H C H H H H H H H C H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	Natura [core] 2S ([core] 2S ([core] 2S (1S (1S (1S (1S (1S (1S ([core] 2S (1S (1S (1S (1S (1S (1S (1S (1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 1.01)2p(3 0.81) 0.78) 0.78) 0.78) 0.78) 0.78) 0.97)2p(3 0.79) 0.79) 0.79) 1.32)2p(4 1.01)2p(3 0.81) 0.79) 1.32)2p(4 1.01)2p(3 0.81) 0.76)	Configuratio	on))))		
	Atom Li N C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H H C H H H H C H H H H C H H H H C H H H H C H H H H H C H H H H H C H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	Natura [core] 2S ([core] 2S ([core] 2S ([core] 2S (1S (1S (1S (1S (1S ([core] 2S (1S (1S ([core] 2S (1S (1S (1S (1S (1S (1S (1S (1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.81) 1.01)2p(3 0.78) 0.78) 0.78) 0.78) 0.78) 0.97)2p(3 0.79) 0.79) 1.32)2p(4 1.01)2p(3 0.79) 1.32)2p(4 1.01)2p(3 0.81) 0.76) 0.79)	Configuratio	on))))		
	Atom Li N C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H C H H C H H C H H H C H C H H C H C H H C H C H H C H C H C H H C H L C H C H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22	Natura [core] 2S ([core] 2S ([core] 2S ([core] 2S (1S (1S (1S (1S (1S ([core] 2S (1S (1S ([core] 2S (1S (1S (1S (1S (1S (1S (1S (1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.97)2p(3 0.79) 0.79) 1.32)2p(4 1.01)2p(3 0.81) 0.76) 0.79) 1.01)2p(3 0.79) 0.79] 0.7	Configuration	on)))))		
	Atom Li N C H H H C H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23	Natura [core]2S([core]2S([core]2S([sore]2S(1S(1S(1S(1S([core]2S(1S(1S([core]2S(1S(1S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.97)2p(3 0.79) 0.80) 0.97)2p(3 0.79) 1.32)2p(4 1.01)2p(3 0.79) 1.32)2p(3 0.79) 1.32)2p(3 0.79) 1.32)2p(3 0.79) 1.32)2p(3 0.79) 1.32)2p(3 0.79) 1.32)2p(3 0.79) 1.32)2p(3 0.79) 1.32)2p(3 0.79) 1.01)2p(3 0.79)2p	Configuration	on))))		
	Atom Li N C H H H C H H H C H H H C H H H C H H H C H H H T H H C H H	No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 55 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 10 25 10 10 10 10 10 10 10 10 10 10	Natura [core] 2S ([core] 2S ([core] 2S ([core] 2S (1S (1S (1S (1S (1S (1S (1S (1	al Electron 0.09)3d(0 1.31)2p(4 1.01)2p(3 0.78) 0.79) 0.81) 1.01)2p(3 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.78) 0.79) 0.79) 1.32)2p(3 0.79) 0.79) 1.32)2p(4 1.01)2p(3 0.79) 1.32)2p(4 1.01)2p(3 0.79)2p(Configuration	on))))		_

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С	26	[core]2S(0.88)2p(3.14)3p(0.01)4p(0.01)
С	27	[core]2S(0.92)2p(3.56)4p(0.03)
Η	28	1S (0.80)	-	
С	29	[core]2S(0.93)2p(3.37)4p(0.02)
Η	30	1S (0.80)		
С	31	[core]2S(0.93)2p(3.38)4p(0.02)
Η	32	1S (0.80)		
С	33	[core]2S(0.92)2p(3.55)4p(0.02)
Η	34	1S (0.80)		
Li	35	[core]2S(0.09)3d(0.01)4p(0.01)
Ν	36	[core]2S(1.31)2p(4.25)4p(0.01)
С	37	[core]2S(1.01)2p(3.40)4p(0.01)
Η	38	1S (0.78)		
Η	39	1S (0.79)		
Η	40	1S (0.81)		
С	41	[core]2S(1.01)2p(3.39)4p(0.01)
Η	42	1S (0.81)		
Η	43	1S (0.78)		
Η	44	1S (0.78)		
С	45	[core]2S(0.97)2p(3.24)4p(0.01)
Η	46	1S (0.78)		
Η	47	1S (0.80)		
С	48	[core]2S(0.97)2p(3.24)4p(0.01)
Η	49	1S (0.79)		
Η	50	1S (0.79)		
Ν	51	[core]2S(1.32)2p(4.26)4p(0.01)
С	52	[core]2S(1.01)2p(3.39)4p(0.01)
Η	53	1S (0.81)		
Η	54	1S (0.76)		
Η	55	1S (0.79)		
С	56	[core]2S(1.01)2p(3.39)4p(0.01)
Η	57	1S (0.79)		
Η	58	1S (0.76)		
Η	59	1S (0.81)		
С	60	[core]2S(0.88)2p(3.15)3p(0.01)4p(0.01)
С	61	[core]2S(0.92)2p(3.58)4p(0.04)
Η	62	1S (0.80)		
С	63	[core]2S(0.93)2p(3.26)3p(0.01)
Η	64	1S (0.82)		
С	65	[core]2S(0.93)2p(3.40)4p(0.03)
Η	66	1S (0.80)		
С	67	[core]2S(0.92)2p(3.55)4p(0.02)
Η	68	1S (0.80)		

1 |1 |UNPC-UNK|SP|RB3LYP|6-31+G(d,p)|C22H40Li2N4|PCUSER|28-Aug-2008|0||# B3LYP/6-31+G(D,P) POP=(NBO,FULL) GEOM=CONNECTIVITY INT=ULTRAFINE SCF= TIGHT||Single point on 2||0,1|Li|N,1,2.12275239|C,2,1.4592254 3,1,106.58359672|H,3,0.95993404,2,109.47987106,1,68.7306377,0|H,3,0.95 978992,2,109.45930829,1,-51.24126721,0|H,3,0.95990392,2,109.46293755,1 ,-171.2879933,0|C,2,1.45677212,1,116.24538622,3,122.11570946,0|H,7,0.9 5997646,2,109.50539566,1,178.57829491,0|H,7,0.9598592,2,109.5146923,1, 58.50375648,0|H,7,0.96069526,2,109.47933752,1,-61.46509045,0|C,2,1.468 89305,1,103.84294701,3,-117.11645077,0|H,11,0.97023252,2,109.20467954, 1,-79.46092451,0|H,11,0.96968767,2,109.20598111,1,162.69895523,0|C,11, 1.50920707,2,111.99365366,1,41.60879241,0|H,14,0.96990107,11,109.37569 001,2,66.31393929,0|H,14,0.96955258,11,109.33417399,2,-175.61174162,0| N,14,1.46397451,11,111.31579847,2,-54.66721341,0|C,17,1.46333286,14,11 0.91788568,11,-78.12473783,0|H,18,0.95972205,17,109.47692249,14,-59.50

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3041,17,109.48165817,14,60.4845624,0 C,17,1.46103898,14,110.03736109,1 1,160.73763118,0|H,22,0.96023482,17,109.50323596,14,-59.76055302,0|H,2 2,0.96017707,17,109.43923217,14,-179.75373608,0 | H,22,0.96006393,17,109 .48198252,14,60.24861259,0|C,1,2.61216876,2,145.37721711,7,-28.2831971 4,0 | C,26,1.42140755,1,61.8640062,2,45.90731574,0 | H,27,0.93007073,26,11 9.39920175,1,-115.26555427,0 C,27,1.43412045,26,121.23681398,1,64.7663 6099,0 | H,29,0.93047313,27,120.21929297,26,164.8650778,0 | C,29,1.3628367 1,27,119.52559339,26,-15.13703593,0 H,31,0.92983066,29,120.37102273,27 ,-179.01109211,0 C,31,1.43624804,29,119.32314263,27,0.97132326,0 H,33, 0.92987985,31,119.29773231,29,-166.29894867,0|Li,26,2.60977624,1,147.6 3983696,2,-179.47269208,0 N,35,2.12275239,26,177.71876604,1,-7.5485209 8,0 | C,36,1.45922543,35,106.58359672,26,157.50758299,0 | H,37,0.95993404, 36,109.47987106,35,-68.7306377,0|H,37,0.95978992,36,109.45930829,35,51 .24126721,0|H,37,0.95990392,36,109.46293755,35,171.2879933,0|C,36,1.45 677212,35,116.24538622,26,35.39187353,0|H,41,0.95997646,36,109.5053956 6,35,-178.57829491,0|H,41,0.9598592,36,109.5146923,35,-58.50375648,0|H ,41,0.96069526,36,109.47933752,35,61.46509045,0|C,36,1.46889305,35,103 .84294701,26,-85.37596623,0 H,45,0.97023252,36,109.20467954,35,79.4609 2451,0|H,45,0.96968767,36,109.20598111,35,-162.69895523,0|C,45,1.50920 707,36,111.99365366,35,-41.60879241,0|H,48,0.96990107,45,109.37569001, 36, -66.31393929, 0 H, 48, 0.96955258, 45, 109.33417399, 36, 175.61174162, 0 N, 48,1.46397451,45,111.31579847,36,54.66721341,0 C,51,1.46333286,48,110. 91788568,45,78.12473783,0 | H,52,0.95972205,51,109.47692249,48,59.506677 39,0|H,52,0.95978967,51,109.48126841,48,179.5447939,0|H,52,0.96033041, 51,109.48165817,48,-60.4845624,0 | C,51,1.46103898,48,110.03736109,45,-1 60.73763118,0|H,56,0.96023482,51,109.50323596,48,59.76055302,0|H,56,0. 96017707,51,109.43923217,48,179.75373608,0 | H,56,0.96006393,51,109.4819 8252,48,-60.24861259,0 C,33,1.41420858,31,121.45757832,29,13.7272786,0 C,60,1.42140755,33,124.60868346,31,166.05739581,0|H,61,0.93007073,60, 119.39920175,33,-14.40723538,0 C,61,1.43412045,60,121.23681398,33,165. 56084937,0|H,63,0.93047313,61,120.21929297,60,-164.8650778,0|C,63,1.36 283671,61,119.52559339,60,15.13703593,0|H,65,0.92983066,63,120.3710227 3,61,179.01109211,0 C,26,1.41420858,1,136.98552198,2,-65.86852632,0 H, 67,0.92987985,26,119.24468425,1,98.16379666,0|| Version=IA32L-G03RevC.02|State=1-AG|HF=-1095.9462555|RMSD=8.141e-009|Dipole=0.,0.,0.|PG=C I [X(C22H40Li2N4)] | @

2.5.B3LYP/6-311++G(d,p)

			Natural Population				
Atom	No	Charge	Core	Valence	Rydberg	Total	
Li	1	0.84988	1.99894	0.11859	0.03260	2.15012	
N	2	-0.57579	1.99956	5.54882	0.02740	7.57579	
С	3	-0.31998	1.99900	4.30984	0.01114	6.31998	
Н	4	0.18643	0.00000	0.81137	0.00219	0.81357	
Н	5	0.17547	0.00000	0.82293	0.00160	0.82453	
Н	6	0.15638	0.00000	0.84152	0.00210	0.84362	
С	7	-0.31048	1.99900	4.30104	0.01044	6.31048	
Н	8	0.15351	0.00000	0.84461	0.00188	0.84649	
Н	9	0.18040	0.00000	0.81797	0.00162	0.81960	
Н	10	0.18436	0.00000	0.81388	0.00176	0.81564	
С	11	-0.14146	1.99892	4.12847	0.01407	6.14146	
Н	12	0.17505	0.00000	0.82306	0.00190	0.82495	
Н	13	0.15942	0.00000	0.83831	0.00227	0.84058	

С	14	-0.14183	1.99893	4.12908	0.01381	6.14183
Н	15	0.17043	0.00000	0.82768	0.00188	0.82957
Н	16	0.16340	0.00000	0.83436	0.00224	0.83660
N	17	-0.57758	1.99956	5.55441	0.02361	7.57758
С	18	-0.31925	1.99898	4.30966	0.01060	6.31925
Н	19	0.15279	0.00000	0.84518	0.00204	0.84721
Н	20	0.20923	0.00000	0.78856	0.00220	0.79077
Н	21	0.17241	0.00000	0.82604	0.00156	0.82759
С	22	-0.31297	1.99898	4.30361	0.01038	6.31297
Н	23	0.17184	0.00000	0.82684	0.00132	0.82816
н	24	0.20281	0.00000	0.79556	0.00163	0.79719
н	25	0.15182	0.00000	0.84643	0.00175	0.84818
С	26	-0.04932	1.99910	4.02722	0.02299	6.04932
С	27	-0.48247	1.99908	4.44576	0.03764	6.48247
H	28	0.16119	0.00000	0.83628	0.00252	0.83881
С	29	-0.28036	1.99919	4.25728	0.02389	6.28036
H	30	0.15788	0.00000	0.83988	0.00224	0.84212
C	31	-0.28986	1,99919	4,26624	0.02442	6.28986
н Н	32	0 15931	0 00000	0 83866	0 00203	0 84069
C	33	-0 46236	1 99907	4 42930	0 03399	6 46236
с Н	34	0 16039	0 00000	0 83693	0 00268	0 83961
T.i	35	0 84847	1 99894	0 11858	0 03401	2 15153
N	36	-0 57592	1 99956	5 54878	0 02758	7 57592
C	37	-0.32000	1 99900	4 30986	0 01114	6 32000
с ч	38	0.18643		0 81138	0 00220	0.92000
н	20	0 17547	0 00000	0 82293	0.00160	0 82453
и П	10	0.15638	0.00000	0.02255	0.00100	0.02400
C	40 41	-0 31048	1 99900	4 30105	0 01044	6 31048
с ч	42	0.15351		9.30103	0.0188	0.91649
и П	13	0.13331	0.00000	0.81797	0.00163	0.81960
п ц	43	0.10040	0.00000	0.01797	0.00102	0.81960
п С	44	0.10430	1 00000	1 12046	0.00170	6 14145
U U	45	-0.14145	1.99092	4.12040	0.01408	0.14145
п	40	0.17504	0.00000	0.02300	0.00190	0.02490
п	4 /	0.15942	1 00000	0.03031 4 12000	0.00227	0.04050
U U	40	-0.14165	1.99093	4.12900	0.01302	0.14103
п	49	0.1/043	0.00000	0.02/00	0.00188	0.02957
H	50	0.16340	1.00000	0.83436	0.00224	0.83660
N C	5 T	-0.57762	1.99956	2.22444	0.02362	7.57762
	5∠ ⊑ 2	-0.31927	1.99898	4.30965	0.01063	0.31927
н	53	0.15278	0.00000	0.84518	0.00204	0.84722
н	54	0.20921	0.00000	0.78856	0.00224	0.79079
П	55	0.17240	1.00000	0.82604	0.00156	0.82760
	50	-0.31298	1.99898	4.30362	0.01038	0.31298
н	57	0.1/184	0.00000	0.82684	0.00132	0.82816
н	20	0.20280	0.00000	0.79556	0.00164	0.79720
H	59	0.15182	0.00000	0.84643	0.00175	0.84818
C	60	-0.04033	1.99908	4.01863	0.02263	6.04033
C	61	-0.48243	1.99908	4.445/3	0.03/63	6.48243
H	62	0.16116	0.00000	0.83632	0.00253	0.83884
U 11	63		т.ааата	4.25/29	0.023/4	0.20022
H	64 CF	0.15/83	0.00000	0.83988	0.00229	0.84217
C	65	-0.29482	1.99921	4.27077	0.02483	6.29482
H	66	0.15926	0.00000	0.83865	0.00209	0.84074
	67	-0.44427	T.998/9	4.41158	0.03390	6.44427
Н	68	0.12820	0.00000	0.83861	0.00289	0.84150
==========	:====			140 25060	=======================================	
^ TOTA	i⊥ *	0.00000	55.9/4/1	149.35068	U.6/461	206.00000

Natural Population

Core

-----55.97471 (99.9548% of 56)

Valence 149.35068 (99.5671% of 150) Natural Minimal Basis 205.32539 (99.6725% of 206) Natural Rydberg Basis 0.67461 (0.3275% of 206) _____ [core]2S(0.12)3d(0.01)4p(0.02)5p(0.01) [core]2S(1.31)2p(4.23)3p(0.01)4p(0.01) [core]2S(0.97)2p(3.34)27' 1S(0.01) Atom No _ _ Li 1 N 2 С 3 H 4

 1S(0.82)

 H
 6

 1S(0.84)

 C
 7

 [core]2S(0.97)2p(3.33)

 H
 8

 1S(0.84)

 1S(0.82)

 10
 1S(0.81)

 11
 [core]2S(0.94)2p(3.19)3p(0.01)

 12
 1S(0.82)

 13
 1S(0.84)

 14
 [core]2S(0.94)2p(3.19)3p(0.01)

 15
 1S(0.83)

 16

 Н H 10 С Н Н С C 14 H 15 15(0.83)N 17 [core] 25(1.32) 2p(4.24) 4p(0.01)C 18 [core] 25(0.97) 2p(3.34)H 19 15(0.85)H 20 15(0.79)H 21 15(0.83)C 22 [core] 25(0.97) 2p(3.34)H 23 15(0.83)H 24 15(0.83)H 24 15(0.83)H 24 15(0.86)H 25 C 26[core] 25(0.90) 2p(3.15) 4p(0.01)C 27 [core] 25(0.91) 2p(3.35) 4p(0.02)H 30 15(0.84)C 31 [core] 25(0.91) 2p(3.35) 4p(0.02)H 30 15(0.84)C 31 [core] 25(0.90) 2p(3.53) 3p(0.01) 4p(0.02)H 32 15(0.84)C 33 [core] 25(0.12) 3d(0.01) 4p(0.02) 5p(0.01)H 34 15(0.84)C 35 [core] 25(0.12) 3d(0.01) 4p(0.02) 5p(0.01)N 36 [core] 25(0.97) 2p(3.34) 3p(0.01) 4p(0.01)C 37 [core] 25(0.97) 2p(3.34) 3p(0.01)H 39 15(0.84)H 39 15(0.84)H 39 15(0.84)H 39 15(0.84)H 39 15(0.84)H 39 15(0.84)H 39 15(0.84)Η
 1S(0.84)

 41
 [core] 2S(0.97) 2p(3.33)

 42
 1S(0.84)
 Η С Н Η 43 1S(0.82)
 1S(0.81)

 45
 [core]2S(0.94)2p(3.19)3p(0.01)

 46
 1S(0.82)
 Η С Η Η 47 1S(0.84) H 47 1S(0.84) C 48 [core]2S(0.94)2p(3.19)3p(0.01) H 49 1S(0.83) H 50 1S(0.83) N 51 [core]2S(1.32)2p(4.24)4p(0.01) C 52 [core]2S(0.97)2p(3.34) H 53 1S(0.85)

Н	54	1S (0.79)			
Н	55	1S (0.83)			
С	56	[core]2S(0.97)2p(3.34)		
Н	57	1S (0.83)			
Η	58	1S (0.80)			
Н	59	1S (0.85)			
С	60	[core]2S(0.87)2p(3.14)4p(0.01)	
С	61	[core]2S(0.90)2p(3.55)4p(0.03)	
Η	62	1S (0.84)			
С	63	[core]2S(0.91)2p(3.35)4p(0.02)	
Η	64	1S (0.84)			
С	65	[core]2S(0.91)2p(3.36)4p(0.02)	
Η	66	1S (0.84)			
С	67	[core]2S(0.88)2p(3.53)3p(0.01)4p(0.02)
Η	68	1S (0.84)			

NBO analysis skipped by request.

1 | 1 | UNPC-UNK | SP | RB3LYP | 6-311++G(d,p) | C22H40Li2N4 | PCUSER | 03-Sep-2008 | 0 | # B3LYP/6-311++G(D,P) POP=(NPA,FULL) GEOM=CONNECTIVITY SCF=TIGHT INT= ULTRAFINE || Single point on 2 || 0,1 |Li |N,1,2.12275239 | C,2,1.45922543,1 ,106.58359672|H,3,0.95993404,2,109.47987106,1,68.7306377,0|H,3,0.95978 992,2,109.45930829,1,-51.24126721,0|H,3,0.95990392,2,109.46293755,1,-1 71.2879933,0 C,2,1.45677212,1,116.24538622,3,122.11570946,0 H,7,0.9599 7646,2,109.50539566,1,178.57829491,0 | H,7,0.9598592,2,109.5146923,1,58. 50375648,0|H,7,0.96069526,2,109.47933752,1,-61.46509045,0|C,2,1.468893 05,1,103.84294701,3,-117.11645077,0|H,11,0.97023252,2,109.20467954,1,-79.46092451,0|H,11,0.96968767,2,109.20598111,1,162.69895523,0|C,11,1.5 0920707,2,111.99365366,1,41.60879241,0 | H,14,0.96990107,11,109.37569001 ,2,66.31393929,0|H,14,0.96955258,11,109.33417399,2,-175.61174162,0|N,1 4,1.46397451,11,111.31579847,2,-54.66721341,0 C,17,1.46333286,14,110.9 1788568,11,-78.12473783,0|H,18,0.95972205,17,109.47692249,14,-59.50667 739,0 | H,18,0.95978967,17,109.48126841,14,-179.5447939,0 | H,18,0.9603304 1,17,109.48165817,14,60.4845624,0 C,17,1.46103898,14,110.03736109,11,1 60.73763118,0 | H,22,0.96023482,17,109.50323596,14,-59.76055302,0 | H,22,0 .96017707,17,109.43923217,14,-179.75373608,0 | H,22,0.96006393,17,109.48 198252,14,60.24861259,0 C,1,2.61216876,2,145.37721711,7,-28.28319714,0 C, 26, 1.42140755, 1, 61.8640062, 2, 45.90731574, 0 H, 27, 0.93007073, 26, 119.3 9920175,1,-115.26555427,0 | C,27,1.43412045,26,121.23681398,1,64.7663609 9,0|H,29,0.93047313,27,120.21929297,26,164.8650778,0|C,29,1.36283671,2 7,119.52559339,26,-15.13703593,0|H,31,0.92983066,29,120.37102273,27,-1 79.01109211,0 | C,31,1.43624804,29,119.32314263,27,0.97132326,0 | H,33,0.9 2987985,31,119.29773231,29,-166.29894867,0|Li,26,2.60977624,1,147.6398 3696,2,-179.47269208,0 N,35,2.12275239,26,177.71876604,1,-7.54852098,0 C,36,1.45922543,35,106.58359672,26,157.50758299,0 H,37,0.95993404,36, 109.47987106,35,-68.7306377,0 H,37,0.95978992,36,109.45930829,35,51.24 126721,0 | H, 37, 0.95990392, 36, 109.46293755, 35, 171.2879933,0 | C, 36, 1.45677 212,35,116.24538622,26,35.39187353,0 H,41,0.95997646,36,109.50539566,3 5,-178.57829491,0|H,41,0.9598592,36,109.5146923,35,-58.50375648,0|H,41 ,0.96069526,36,109.47933752,35,61.46509045,0 C,36,1.46889305,35,103.84 294701,26,-85.37596623,0 | H,45,0.97023252,36,109.20467954,35,79.4609245 1,0|H,45,0.96968767,36,109.20598111,35,-162.69895523,0|C,45,1.50920707 ,36,111.99365366,35,-41.60879241,0|H,48,0.96990107,45,109.37569001,36, -66.31393929,0 | H,48,0.96955258,45,109.33417399,36,175.61174162,0 | N,48, 1.46397451,45,111.31579847,36,54.66721341,0 C,51,1.46333286,48,110.917 88568,45,78.12473783,0 | H,52,0.95972205,51,109.47692249,48,59.50667739, 0|H,52,0.95978967,51,109.48126841,48,179.5447939,0|H,52,0.96033041,51, 109.48165817,48,-60.4845624,0 C,51,1.46103898,48,110.03736109,45,-160. 73763118,0|H,56,0.96023482,51,109.50323596,48,59.76055302,0|H,56,0.960 17707,51,109.43923217,48,179.75373608,0 | H,56,0.96006393,51,109.4819825 2,48,-60.24861259,0|C,33,1.41420858,31,121.45757832,29,13.7272786,0|C,

60,1.42140755,33,124.60868346,31,166.05739581,0 | H,61,0.93007073,60,119 .39920175,33,-14.40723538,0 | C,61,1.43412045,60,121.23681398,33,165.560 84937,0 | H,63,0.93047313,61,120.21929297,60,-164.8650778,0 | C,63,1.36283 671,61,119.52559339,60,15.13703593,0 | H,65,0.92983066,63,120.37102273,6 1,179.01109211,0 | C,26,1.41420858,1,136.98552198,2,-65.86852632,0 | H,67, 0.92987985,26,119.24468425,1,98.16379666,0 | | Version=IA32L-G03RevC.02 | State=1-AG | HF=-1096.1832043 | RMSD=3.221e-009 | Dipole=0.,0.,0. | PG=CI [X(C22H40Li2N4)] | @

2.6. MP2/LANL2DZ

		NT - to cons - 7		Natural Pop	ulation	
Atom	No	Charge	Core	Valence	Rydberg	Total
Li	1	0.91915	1.99835	0.05909	0.02341	2.08085
Ν	2	-0.58448	1.99971	5.56859	0.01618	7.58448
С	3	-0.29935	1.99927	4.28864	0.01144	6.29935
Н	4	0.18239	0.00000	0.81611	0.00151	0.81761
Н	5	0.16994	0.00000	0.82876	0.00130	0.83006
Н	6	0.14402	0.00000	0.85276	0.00323	0.85598
С	7	-0.28967	1.99927	4.27923	0.01117	6.28967
Н	8	0.14149	0.00000	0.85536	0.00315	0.85851
Н	9	0.17657	0.00000	0.82219	0.00124	0.82343
Н	10	0.18001	0.00000	0.81864	0.00134	0.81999
С	11	-0.12297	1.99919	4.10415	0.01963	6.12297
Н	12	0.16831	0.00000	0.82968	0.00202	0.83169
Н	13	0.14801	0.00000	0.84830	0.00370	0.85199
С	14	-0.12272	1.99920	4.10433	0.01919	6.12272
Н	15	0.16224	0.00000	0.83569	0.00206	0.83776
Н	16	0.15222	0.00000	0.84417	0.00361	0.84778
N	17	-0.59159	1.99971	5.57612	0.01575	7.59159
С	18	-0.29543	1.99925	4.28332	0.01286	6.29543
Н	19	0.14086	0.00000	0.85619	0.00295	0.85914
Н	20	0.20118	0.00000	0.79615	0.00267	0.79882
Н	21	0.16702	0.00000	0.83177	0.00121	0.83298
С	22	-0.29005	1.99925	4.27888	0.01192	6.29005
Н	23	0.16632	0.00000	0.83247	0.00122	0.83368
Н	24	0.19855	0.00000	0.79974	0.00171	0.80145
Н	25	0.13965	0.00000	0.85739	0.00296	0.86035
С	26	-0.00336	1.99914	3.97912	0.02510	6.00336
С	27	-0.52870	1.99919	4.48228	0.04723	6.52870
Н	28	0.15761	0.00000	0.84073	0.00166	0.84239
С	29	-0.26241	1.99932	4.23420	0.02889	6.26241
Н	30	0.14957	0.00000	0.84872	0.00172	0.85043
С	31	-0.27847	1.99932	4.24898	0.03017	6.27847
Н	32	0.15108	0.00000	0.84727	0.00165	0.84892
С	33	-0.50281	1.99918	4.46158	0.04205	6.50281
Н	34	0.15583	0.00000	0.84241	0.00176	0.84417
Li	35	0.91915	1.99835	0.05909	0.02341	2.08085
N	36	-0.58448	1.99971	5.56859	0.01618	7.58448
С	37	-0.29935	1.99927	4.28864	0.01144	6.29935
Н	38	0.18239	0.00000	0.81611	0.00151	0.81761
Н	39	0.16994	0.00000	0.82876	0.00130	0.83006
Н	40	0.14402	0.00000	0.85276	0.00323	0.85598
С	41	-0.28967	1.99927	4.27923	0.01117	6.28967
Н	42	0.14149	0.00000	0.85536	0.00315	0.85851

	н	43	0.17657	0.0000	0.82219	0.00124	0.82343	
	тт тт	11	0 19001	0 00000	0 01064	0 00124	0 91000	
	п	44	0.10001	0.00000	0.01004	0.00134	0.01999	
	C	45	-0.12297	1.99919	4.10415	0.01963	6.12297	
	Н	46	0.16831	0.00000	0.82968	0.00202	0.83169	
	Н	47	0.14801	0.00000	0.84830	0.00370	0.85199	
	C	18	_0 12272	1 99920	1 10133	0 01919	6 12272	
		40	0.12272	1.)))20	4.10455	0.01919	0.12272	
	н	49	0.16224	0.00000	0.83569	0.00206	0.83776	
	H	50	0.15222	0.00000	0.84417	0.00361	0.84778	
	N	51	-0.59159	1.99971	5.57612	0.01575	7.59159	
	С	52	-0.29543	1,99925	4.28332	0.01286	6.29543	
	н	53	0 14086	0 00000	0 85619	0 00295	0 85914	
	11	55	0.14000	0.00000	0.00015	0.00255	0.00014	
	н	54	0.20118	0.00000	0.79615	0.00267	0./9882	
	Н	55	0.16702	0.00000	0.83177	0.00121	0.83298	
	С	56	-0.29005	1.99925	4.27888	0.01192	6.29005	
	Н	57	0.16632	0.00000	0.83247	0.00122	0.83368	
	н	58	0 19855	0 00000	0 79974	0 00171	0 80145	
	11	50	0.12005	0.00000	0.75571	0.00171	0.00115	
	н	59	0.13965	0.00000	0.85739	0.00296	0.86035	
	C	60	-0.00336	1.99914	3.97912	0.02510	6.00336	
	С	61	-0.52870	1.99919	4.48228	0.04723	6.52870	
	Н	62	0.15761	0.00000	0.84073	0.00166	0.84239	
	С	63	-0 26241	1 99932	4 23420	0 02889	6 26241	
	U U	61	0 1/957	0 00000	0 0/072	0 00172	0 95043	
	п	64	0.14957	0.00000	0.04072	0.00172	0.85045	
	C	65	-0.27847	1.99932	4.24898	0.03017	6.27847	
	H	66	0.15108	0.00000	0.84727	0.00165	0.84892	
	С	67	-0.50281	1.99918	4.46158	0.04205	6.50281	
	Н	68	0.15583	0.00000	0.84241	0.00176	0.84417	
=		====						
	* Tota	1 *	0 00000	55 97872	149 30598	0 71530	206 00000	
	1004		0.00000	55.57072	140.00000	0.71550	200.00000	
				Natur	al Donulation	n		
				Natur	al Population	n		
-				Natur	al Population	n 		
-	Core			Natur 55.97872	al Populatio (99.9620% o	n f 56)		
-	Core Valenc			Natur 55.97872 149.30598	al Populatio (99.9620% o (99.5373% o	n f 56) f 150)		
-	Core Valenc Natura	e 1 Min	nimal Basis	Natur 55.97872 149.30598 205.28470	al Populatio (99.9620% o (99.5373% o (99.6528% o	n f 56) f 150) f 206)		
_	Core Valenc Natura Natura	e 1 Min	nimal Basis lberg Basis	Natur 55.97872 149.30598 205.28470 0.71530	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o	n f 56) f 150) f 206) f 206)		
_	Core Valenc Natura Natura	e 1 Min 1 Ryc	nimal Basis Aberg Basis	Natur 55.97872 149.30598 205.28470 0.71530	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o	n f 56) f 150) f 206) f 206)		
_	Core Valenc Natura Natura	e 1 Min 1 Ryc	nimal Basis dberg Basis	Natur 55.97872 149.30598 205.28470 0.71530	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o	n f 56) f 150) f 206) f 206)		
_	Core Valenc Natura Natura Atom	e 1 Min 1 Ryc 	nimal Basis dberg Basis Natur	Natur 55.97872 149.30598 205.28470 0.71530	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o 	n f 56) f 150) f 206) f 206) 		
_	Core Valenc Natura Natura Atom	ee l Min l Rya No	nimal Basis lberg Basis Natur	Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati	n f 56) f 150) f 206) f 206) 		_
_	Core Valenc Natura Natura Atom	e l Min l Ryd No	nimal Basis lberg Basis Natur	Natur 55.97872 149.30598 205.28470 0.71530 al Electron	al Populatio (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati	n f 56) f 150) f 206) f 206) 		_
-	Core Valenc Natura Natura Atom	e l Min l Ryd No	nimal Basis lberg Basis Natur	Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configuration	n f 56) f 150) f 206) f 206) 		_
-	Core Valenc Natura Natura Atom Li	e l Min l Ryc No	nimal Basis lberg Basis Natur [core]2S(Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o 	n f 56) f 150) f 206) f 206) 		_
-	Core Valenc Natura Natura Atom Li N	e l Min l Ryc No l 2	nimal Basis lberg Basis Natur [core]2S([core]2S(Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o 	n f 56) f 150) f 206) f 206) 		
-	Core Valenc Natura Natura Atom Li N C	e l Min l Ryc No 1 2 3	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o 	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H	e l Min l Ryc No 1 2 3 4	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o 	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H H	ee 1 Min 1 Ryo No 1 2 3 4 5	nimal Basis lberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o 	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H H H	ee 1 Min 1 Ryo No 1 2 3 4 5 6	nimal Basis lberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o 	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H H H C	ee 1 Min 1 Rya No 1 2 3 4 5 6 7	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configuration .02) .22)3p(0.02 .30)3p(0.01	n f 56) f 150) f 206) f 206) 		_
-	Core Valenc Natura Natura Atom Li N C H H H H C U	ee 1 Min 1 Rya No 1 2 3 4 5 6 7 8	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.83) 0.85) 0.98)2p(3	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configuration .02) .22)3p(0.02 .30)3p(0.01	n f 56) f 150) f 206) f 206) on 		
-	Core Valenc Natura Natura Atom Li N C H H H C H	ee l Min l Ryd NO 1 2 3 4 5 6 7 8	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.83) 0.85) 0.98)2p(3 0.86) 2.26(1)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configuration .02) .22)3p(0.02 .30)3p(0.01	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H H H H C H H H	ee l Min l Ryd 1 2 3 4 5 6 7 8 9	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.83) 0.85) 0.98)2p(3 0.86) 0.82)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H H H H H H H H H	ee 1 Min 1 Ryd 1 2 3 4 5 6 7 8 9 10	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.83) 0.85) 0.98)2p(3 0.85) 0.98)2p(3 0.82) 0.82) 0.82)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H H H H C H H H C H H H C	ee 1 Min 1 Ryd No 1 2 3 4 5 6 7 8 9 10 11	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(2S(1S(2S(2S(2S(2S(2S(2S(2S(2S(2S(2	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.83) 0.85) 0.98)2p(3 0.82) 0.96)220(3)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H H H H C H H H C H H	ee 1 Min 1 Ryd NO 1 2 3 4 5 6 7 8 9 10 11 12	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.83) 0.85) 0.98)2p(3 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.83)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H H H H C H H H H C H H H	ee 1 Min 1 Ryd NO 1 2 3 4 5 6 7 8 9 10 11 12 13	nimal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.83) 0.85) 0.98)2p(3 0.82) 0.83) 0.85)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01	n f 56) f 150) f 206) f 206) on 		_
-	Core Valenc Natura Natura Atom Li N C H H H C H H H C H H H C H H H C H H C H H C H H C H H C H H C C H	ee 1 Min 1 Ryd NO 1 2 3 4 5 6 7 8 9 10 11 12 13 14	himal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.82) 0.83) 0.85) 0.98)2p(3 0.82)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01 .15)3p(0.02	n f 56) f 150) f 206) f 206) on)))		_
	Core Valenc Natura Natura Atom Li N C H H H C H H H C H H H C H H H C C H H C H H C C H	ee l Min l Ryd No l 2 3 4 5 6 7 8 9 10 11 12 13 14 	himal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.82) 0.82) 0.85) 0.98)2p(3 0.82) 0.82) 0.82) 0.82) 0.82) 0.85) 0.96)2p(3 0.85) 0.95)2p(3 0.95)2p(3) 0.95)2p(3) 0.95)2p(3) 0.95)2p(3)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01 .15)3p(0.02 .15)3p(0.02	n f 56) f 150) f 206) f 206) on)))		_
	Core Valenc Natura Natura Atom Li N C H H H C H H H C H H H C H H H C H H	ee l Min l Ryd No l 2 3 4 5 6 7 8 9 10 11 12 13 14 15	himal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.82) 0.85) 0.98)2p(3 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.85) 0.96)2p(3 0.83) 0.85) 0.95)2p(3 0.84) 0.84)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01 .15)3p(0.02 .15)3p(0.02	n f 56) f 150) f 206) f 206) on)))		
-	Core Valenc Natura Natura Atom Li N C H H H C H H H C H H H C H H H C H H H H C H H H H C H H H H C H H H H	ee l Min l Ryd No l 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	himal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.82) 0.85) 0.98)2p(3 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.96)2p(3 0.82) 0.83) 0.85) 0.95)2p(3) 0.84) 0.84)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01 .15)3p(0.02 .15)3p(0.02	n f 56) f 150) f 206) f 206) on)))		_
-	Core Valenc Natura Natura Atom Li N C H H H C H H H C H H H C H H H N C	ee l Min l Ryd No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	himal Basis dberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.95)2p(3) 0.84) 1.35)2p(4)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01 .15)3p(0.02 .15)3p(0.02 .23)3p(0.02	n f 56) f 150) f 206) f 206) on))))		_
	Core Valenc Natura Atom Li N C H H H C H H H C H H H C H H H C H H H C H H H C C H H H C C H H H C C H H C C H H C C H C H C H C H C H C H C C H C C H C C H C C H C C H C C H C C H C C H C C H C	ee l Min l Ryd No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	nimal Basis lberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.96)2p(3 0.82) 0.95)2p(3 0.82) 0.95)2p(3 0.82) 0.95)2p(3 0.82) 0.95)2p(3 0.82) 0.95)2p(3 0.82) 0.95)2p(3 0.82) 0.95)2p(3 0.82) 0.95)2p(3 0.82) 0.95)2p(3 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.95)2p(3 0.82) 0.82) 0.82) 0.82) 0.95)2p(3 0.82)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01 .15)3p(0.02 .15)3p(0.02 .23)3p(0.02 .30)3p(0.01	n f 56) f 150) f 206) f 206) on))))		_
_	Core Valenc Natura Natura Atom Li N C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H H C H H H H C H H H H H C H	ee 1 Min 1 Rya No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	nimal Basis lberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 al Electron 0.06)3p(0 1.34)2p(4 0.98)2p(3 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.82) 0.96)2p(3 0.82) 0.82) 0.96)2p(3 0.82) 0.96)2p(3 0.83) 0.85) 0.95)2p(3 0.84) 0.84) 1.35)2p(4 0.98)2p(3 0.84) 0.84) 1.35)2p(4 0.98)2p(3 0.86)	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .22)3p(0.02 .30)3p(0.01 .30)3p(0.01 .15)3p(0.02 .15)3p(0.02 .23)3p(0.02 .30)3p(0.01	n f 56) f 150) f 206) f 206) on))))		_
-	Core Valenc Natura Natura Atom Li N C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H H C H H H H C H H H H C H	ee 1 Min 1 Rya No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	nimal Basis lberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S([core]2S(1S(1S(1S([core]2S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .02) .22)3p(0.02 .30)3p(0.01 .30)3p(0.01 .15)3p(0.02 .15)3p(0.02 .23)3p(0.02 .30)3p(0.01	n f 56) f 150) f 206) f 206) f 206) on))))		
-	Core Valenc Natura Natura Atom Li N C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H C H H H H C H H H H C H	ee 1 Min 1 Rya No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21	nimal Basis lberg Basis Natur [core]2S([core]2S([core]2S(1S(1S(1S(1S(1S([core]2S(1S(1S(1S(1S(1S(1S(1S(1	Natur 55.97872 149.30598 205.28470 0.71530 	al Population (99.9620% o (99.5373% o (99.6528% o (0.3472% o Configurati .22)3p(0.02 .30)3p(0.01 .30)3p(0.01 .15)3p(0.02 .15)3p(0.02 .23)3p(0.02 .30)3p(0.01	n f 56) f 150) f 206) f 206) f 206) on))))		_

C H H	22 23 24	[core]2S(1S(1S(0.98)2p(0.83) 0.80)	3.30)3p(0.01)
п	25	JS((0.86)	2 00 2 m	0 0 0 0 0
C	26	[core]2S(0.90)2p(3.08)3p((0.02)
	27		0.92)2p(3.20/30(0.05)
п	20) GL	0.84)	2 20 2 m	0 0 2)
	29		0.93)2p(3.30)3p(0.03)
Н	30	LS((0.85)	2 21 2 - (0 0 2)
	31	[core]2S(0.93)2p(3.31)3p(0.03)
н	3∠ 22	LS ((0.85)	$2 = 4 \setminus 2 = 6$	0 04)
	33	[core]2S(0.92)2p(3.54)3p(0.04)
п т :	34	LS((0.84)	0 0 0 0	
Ll	35	[core]2S(0.06)3p(0.02)	0 00)
N	36	[core]2S(1.34)2p(4.22)3p((0.02)
	37	[core]2S(0.98)2p(3.30)3p(0.01)
H	38	1S((0.82)		
H	39	1S (0.83)		
H	40	IS(0.85)	2 20)2 (0 01)
C	41	[core]2S(0.98)2p(3.30)3p(0.01)
H	42	1S(0.86)		
H	43	IS(0.82)		
H	44	1S(0.82)	2 1 5 2 (0 00)
C	45	[core]2S(0.96)2p(3.15)3p(0.02)
H	46	1S(0.83)		
H	4 /	IS(0.85)	2 1 5 2 (0 00)
C	48	[core]2S(0.95)2p(3.15)3p(0.02)
H	49	1S(0.84)		
H	50	IS((0.84)	4 22)200(0 00)
N	51	[core]2S(1.35)2p(4.23)3p((0.02)
C	52	[core]2S(0.98)2p(3.30)3p(0.01)
H	53	1S(0.86)		
H	54	1S(0.80)		
Н	55	IS((0.83)	2 20	0 01)
	56	[core]2S(0.98)2p(3.30)3p(0.01)
H	57	1S(0.83)		
H	58	IS (0.80)		
H	59	IS(0.86)	2 0 0) 2 - (0 00)
C	60	[core]2S(0.90)2p(3.08)3p((0.02)
C	61	[core]2S(0.92)2p(3.56)3p(0.05)
H	62	LS((0.84)		0 02
C.	63	[core]2S(0.93)2p(3.30)3p(0.03)
H	64	1S(0.85)	2 21/2 (0 0 0 1
C	65	[core]2S(0.93)2p(з.зт)зр(0.03)
H	66		0.85)		0.01
C	67	[core]2S(0.92)2p(3.54)3p(0.04)
Ĥ	68	1S(0.84)		

NBO analysis skipped by request.

1 | 1 | UNPC-UNK | SP | RMP2-FU | LANL2DZ | C22H40Li2N4 | PCUSER | 02-Sep-2008 | 0 | | # MP 2=FULL/LANL2DZ POP= (NPA, FULL) GEOM=CONNECTIVITY SCF=TIGHT INT=ULTRAFIN E | Single point on 2 | 0,1 | Li | N,1,2.12275239 | C,2,1.45922543,1,106.583 59672 | H,3,0.95993404,2,109.47987106,1,68.7306377,0 | H,3,0.95978992,2,10 9.45930829,1,-51.24126721,0 | H,3,0.95990392,2,109.46293755,1,-171.28799 33,0 | C,2,1.45677212,1,116.24538622,3,122.11570946,0 | H,7,0.95997646,2,1 09.50539566,1,178.57829491,0 | H,7,0.9598592,2,109.5146923,1,58.50375648 ,0 | H,7,0.96069526,2,109.47933752,1,-61.46509045,0 | C,2,1.46889305,1,103 .84294701,3,-117.11645077,0 | H,11,0.97023252,2,109.20467954,1,-79.46092 451,0 | H,11,0.96968767,2,109.20598111,1,162.69895523,0 | C,11,1.50920707, 2,111.99365366,1,41.60879241,0 | H,14,0.96990107,11,109.37569001,2,66.31

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393929,0|H,14,0.96955258,11,109.33417399,2,-175.61174162,0|N,14,1.4639 7451,11,111.31579847,2,-54.66721341,0|C,17,1.46333286,14,110.91788568, 11,-78.12473783,0|H,18,0.95972205,17,109.47692249,14,-59.50667739,0|H, 18,0.95978967,17,109.48126841,14,-179.5447939,0|H,18,0.96033041,17,109 .48165817,14,60.4845624,0 C,17,1.46103898,14,110.03736109,11,160.73763 118,0 | H,22,0.96023482,17,109.50323596,14,-59.76055302,0 | H,22,0.9601770 7,17,109.43923217,14,-179.75373608,0 | H,22,0.96006393,17,109.48198252,1 4,60.24861259,0 | C,1,2.61216876,2,145.37721711,7,-28.28319714,0 | C,26,1. 42140755,1,61.8640062,2,45.90731574,0|H,27,0.93007073,26,119.39920175, 1,-115.26555427,0 C,27,1.43412045,26,121.23681398,1,64.76636099,0 H,29 ,0.93047313,27,120.21929297,26,164.8650778,0|C,29,1.36283671,27,119.52 559339,26,-15.13703593,0 H,31,0.92983066,29,120.37102273,27,-179.01109 211,0 C,31,1.43624804,29,119.32314263,27,0.97132326,0 H,33,0.92987985, 31,119.29773231,29,-166.29894867,0|Li,26,2.60977624,1,147.63983696,2,-179.47269208,0 | N,35,2.12275239,26,177.71876604,1,-7.54852098,0 | C,36,1. 45922543,35,106.58359672,26,157.50758299,0|H,37,0.95993404,36,109.4798 7106,35,-68.7306377,0|H,37,0.95978992,36,109.45930829,35,51.24126721,0 |H,37,0.95990392,36,109.46293755,35,171.2879933,0|C,36,1.45677212,35,1 16.24538622,26,35.39187353,0 | H,41,0.95997646,36,109.50539566,35,-178.5 7829491,0|H,41,0.9598592,36,109.5146923,35,-58.50375648,0|H,41,0.96069 526, 36, 109.47933752, 35, 61.46509045, 0 C, 36, 1.46889305, 35, 103.84294701, 2 6,-85.37596623,0|H,45,0.97023252,36,109.20467954,35,79.46092451,0|H,45 ,0.96968767,36,109.20598111,35,-162.69895523,0|C,45,1.50920707,36,111. 99365366,35,-41.60879241,0|H,48,0.96990107,45,109.37569001,36,-66.3139 3929,0 | H,48,0.96955258,45,109.33417399,36,175.61174162,0 | N,48,1.463974 51,45,111.31579847,36,54.66721341,0 C,51,1.46333286,48,110.91788568,45 ,78.12473783,0|H,52,0.95972205,51,109.47692249,48,59.50667739,0|H,52,0 .95978967,51,109.48126841,48,179.5447939,0|H,52,0.96033041,51,109.4816 5817,48,-60.4845624,0 C,51,1.46103898,48,110.03736109,45,-160.73763118 ,0|H,56,0.96023482,51,109.50323596,48,59.76055302,0|H,56,0.96017707,51 ,109.43923217,48,179.75373608,0 | H,56,0.96006393,51,109.48198252,48,-60 .24861259,0 C,33,1.41420858,31,121.45757832,29,13.7272786,0 C,60,1.421 40755,33,124.60868346,31,166.05739581,0 | H,61,0.93007073,60,119.3992017 5,33,-14.40723538,0 C,61,1.43412045,60,121.23681398,33,165.56084937,0 H,63,0.93047313,61,120.21929297,60,-164.8650778,0 | C,63,1.36283671,61,1 19.52559339,60,15.13703593,0 | H,65,0.92983066,63,120.37102273,61,179.01 109211,0 C,26,1.41420858,1,136.98552198,2,-65.86852632,0 H,67,0.929879 85,26,119.24468425,1,98.16379666,0 Version=IA32L-G03RevC.02 State =1-AG|HF=-1088.1227078|MP2=-1090.3693094|RMSD=4.952e-009|PG=CI [X(C22H 40Li2N4)]||@

2.7. MP2/6-31+G(d)

			Natural	Natural Population				
_	Atom	No	Charge	Core	Valence	Rydberg	Total	
	Li	1	0.89105	1.99920	0.08367	0.02609	2.10895	
	Ν	2	-0.65131	1.99961	5.62582	0.02588	7.65131	
	С	3	-0.32278	1.99951	4.30841	0.01486	6.32278	
	Н	4	0.19581	0.00000	0.80257	0.00162	0.80419	
	Н	5	0.18482	0.00000	0.81445	0.00074	0.81518	
	Н	6	0.16578	0.00000	0.83352	0.00070	0.83422	
	С	7	-0.31593	1.99951	4.30195	0.01447	6.31593	
	Н	8	0.16281	0.00000	0.83656	0.00063	0.83719	
	Н	9	0.19091	0.00000	0.80819	0.00090	0.80909	
	Н	10	0.19454	0.00000	0.80452	0.00094	0.80546	

С	11	-0.16092	1.99938	4.14386	0.01768	6.16092
Н	12	0.19390	0.0000	0.80537	0.00073	0.80610
Н	13	0.17582	0.00000	0.82348	0.00070	0.82418
С	14	-0.16005	1.99939	4.14323	0.01742	6.16005
Н	15	0.18822	0.00000	0.81104	0.00075	0.81178
Н	16	0.17943	0.0000	0.81983	0.00074	0.82057
N	17	-0.65631	1.99961	5.63187	0.02483	7.65631
С	18	-0.32121	1.99949	4.30706	0.01467	6.32121
Н	19	0.16178	0.0000	0.83754	0.00068	0.83822
Н	20	0.21885	0.0000	0.78019	0.00096	0.78115
Н	21	0.18159	0.00000	0.81773	0.00068	0.81841
C	22	-0.31768	1.99950	4.30367	0.01451	6.31768
H	23	0.18139	0.0000	0.81807	0.00053	0.81861
H	24	0.21339	0.00000	0.78555	0.00107	0.78661
H	25	0.16058	0.00000	0.83883	0.00059	0.83942
C	26	0.01734	1.99909	3.95555	0.02802	5.98266
C	27	-0.55591	1.99926	4.51566	0.04099	6.55591
H	28	0.18370	0.00000	0.81532	0.00098	0.81630
C	29	-0.28151	1.99931	4.24943	0.03277	6.28151
н	30	0.1/5/0	0.00000	0.82341	0.00089	0.82430
U U	31 22	-0.29622	1.99932	4.20378	0.03313	0.29622
п	2∠ 22	-0 53695	1 99925	0.02203	0.00091	6 52695
с ч	31	0.18233	1.99923	4.49900	0.03870	0.33093
т.і	25	0.10255	1 99920	0.01001	0.00100	2 10895
N	36	-0 65131	1 99961	5 62582	0.02588	7 65131
C	37	-0 32278	1 99951	4 30841	0 01486	6 32278
U H	38	0.19581	0.00000	0.80257	0.00162	0.80419
H	39	0.18482	0.00000	0.81445	0.00074	0.81518
Н	40	0.16578	0.00000	0.83352	0.00070	0.83422
С	41	-0.31593	1.99951	4.30195	0.01447	6.31593
Н	42	0.16281	0.0000	0.83656	0.00063	0.83719
Н	43	0.19091	0.0000	0.80819	0.00090	0.80909
Н	44	0.19454	0.0000	0.80452	0.00094	0.80546
С	45	-0.16092	1.99938	4.14386	0.01768	6.16092
Н	46	0.19390	0.00000	0.80537	0.00073	0.80610
Н	47	0.17582	0.00000	0.82348	0.00070	0.82418
C	48	-0.16005	1.99939	4.14323	0.01742	6.16005
Н	49	0.18822	0.00000	0.81104	0.00075	0.81178
Н	50	0.17943	0.00000	0.81983	0.00074	0.82057
N	51	-0.65631	1.99961	5.63187	0.02483	7.65631
C	52	-0.32121	1.99949	4.30706	0.01467	6.32121
H	53	0.16178	0.00000	0.83754	0.00068	0.83822
н	54	0.21885	0.00000	0.78019	0.00096	0.78115
н	55	0.18159	1.00050	0.81/73	0.00068	0.81841
U U	20 57	-U.31/68	1.99950	4.30367	0.01451	0.31/08
н ч	58	0.10139	0.00000	0.81807	0.000000	0.01001
и Н	59	0.16058	0.00000	0.83883	0 00059	0 83942
C	60	0.01734	1,99909	3,95555	0.02802	5,98266
C	61	-0.55591	1.99926	4.51566	0.04099	6.55591
H	62	0.18370	0.00000	0.81532	0.00098	0.81630
С	63	-0.28151	1.99931	4.24943	0.03277	6.28151
H	64	0.17570	0.00000	0.82341	0.00089	0.82430
С	65	-0.29622	1.99932	4.26378	0.03313	6.29622
Н	66	0.17706	0.00000	0.82203	0.00091	0.82294
С	67	-0.53695	1.99925	4.49900	0.03870	6.53695
Н	68	0.18233	0.00000	0.81661	0.00106	0.81767
=======		=============	=================			
* Tota	al *	0.00000	55.98283	149.29552	0.72165	206.00000

				Natural Population
-	Core Valence Natural Natural	Minimal Rydberg	Basis Basis	55.98283 (99.9693% of 56) 149.29552 (99.5303% of 150) 205.27835 (99.6497% of 206) 0.72165 (0.3503% of 206)
-	Atom 1	No	Natura	al Electron Configuration
-				
	Li	1	[core]2S(0.08)3d(0.01)4p(0.01)
	N	2	[core]2S(1.32)2p(4.31)3d(0.01)4p(0.02)
	с н	3 Д	[COTE]25(19(1.01/2p(3.30/3d(0.01/4p(0.01)))
	H	- 5	15(0.81)
	H	6	1S (0.83)
	С	7	[core]2S(1.01)2p(3.30)3d(0.01)4p(0.01)
	Н	8	1S (0.84)
	Н	9	1S (0.81)
	H I	10	1S(0.80)
	C	11	[core]2S(0.97)2p(3.17)3d(0.01)4p(0.01)
	H 1	12	1S(0.81)
	H I	14	IS((0.82)
	с. ч	14 15	[core]25(0.97)2p(3.18)3d(0.01)4p(0.01)
	н.	16	19(0.82)
	N 1	17	[core]2S(1.32)2p(4.31)3d(0.01)4p(0.01)
	C	18	[core]2S(1.01)2p(3.30)3d(0.01)4p(0.01)
	H I	19	1S (0.84)
	H 2	20	1S (0.78)
	H 2	21	1S (0.82)
	C 2	22	[core]2S(1.01)2p(3.30)3d(0.01)4p(0.01)
	H 2	23	1S (0.82)
	H 2	24	1S(0.79)
	H 2	25	IS((0.84)
		20 27	[core]25((0.88) 2p((3.07) 3p((0.01) 3d((0.01) 4p((0.01))))
	н	2.8	1S(0.32)2p(3.00)4p(0.03)
	C	29	[core]2S(0.92)2p(3.32)3d(0.01)4p(0.02)
	н	30	1S(0.82)
	C 3	31	[core]2S(0.93)2p(3.34)3d(0.01)4p(0.02)
	H C	32	1S (0.82)
	C :	33	[core]2S(0.91)2p(3.59)4p(0.03)
	H S	34	1S(0.82)
	Li :	35	[core]2S(0.08)3d(0.01)4p(0.01)
	N .	36	[core]2S(1.32)2p(4.31)3d(0.01)4p(0.02) 1.01)2p(2.20)2d(0.01)4p(0.01)
	с. ч	2 A 2 B	[COTE]25(19(1.01/2p(3.30/3d(0.01/4p(0.01)))
	Н	39	15(0.81)
	H 4	40	1S (0.83)
	C 4	41	[core]2S(1.01)2p(3.30)3d(0.01)4p(0.01)
	H 4	42	1S (0.84)
	H 4	43	1S (0.81)
	H 4	44	1S(0.80)
	C 4	45	[core]2S(0.97)2p(3.17)3d(0.01)4p(0.01)
	H 4	46 47	1S(U.81)
		4/ 40	LS(U.02
	с 4 ц ,	±0 49	1COTE]25(0.57/2p(5.10)3u(0.01)4p(0.01) 0.81)
	H !	50	15 (1S (0.82)
			(

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Ν	51	[core]2S(1.32)2p(4.31)3d(0.01)4p(0.01)	
С	52	[core]2S(1.01)2p(3.30)3d(0.01)4p(0.01)	
Η	53	1S (0.84)				
Η	54	1S (0.78)				
Η	55	1S (0.82)				
С	56	[core]2S(1.01)2p(3.30)3d(0.01)4p(0.01)	
Η	57	1S (0.82)				
Η	58	1S (0.79)				
Η	59	1S (0.84)				
С	60	[core]2S(0.88)2p(3.07)3p(0.01)3d(0.01)4p(0.01)
С	61	[core]2S(0.92)2p(3.60)4p(0.03)		
Η	62	1S (0.82)				
С	63	[core]2S(0.92)2p(3.32)3d(0.01)4p(0.02)	
Η	64	1S (0.82)				
С	65	[core]2S(0.93)2p(3.34)3d(0.01)4p(0.02)	
Η	66	1S (0.82)				
С	67	[core]2S(0.91)2p(3.59)4p(0.03)		
Η	68	1S (0.82)				

NBO analysis skipped by request.

1 | 1 | UNPC-UNK | SP | RMP2-FC | 6-31+G (d) | C22H40Li2N4 | PCUSER | 04-Sep-2008 | 0 | | # MP2/6-31+G(D) POP=(NPA, FULL) GEOM=CONNECTIVITY SCF=TIGHT INT=ULTRAFINE ||Single point on 2||0,1|Li|N,1,2.12270033|C,2,1.45914083,1,106.5856 5173 |H,3,0.95995951,2,109.48429114,1,68.73082123,0 |H,3,0.95983992,2,10 9.46381677,1,-51.24253335,0|H,3,0.9599558,2,109.46704578,1,-171.287939 55,0 C,2,1.45682816,1,116.2463274,3,122.11622054,0 H,7,0.9598988,2,109 .50801728,1,178.57681344,0 H,7,0.95989617,2,109.51096754,1,58.49938321 ,0|H,7,0.96072409,2,109.47331879,1,-61.4626441,0|C,2,1.46888952,1,103. 84433854,3,-117.11812327,0|H,11,0.97026537,2,109.20627609,1,-79.455592 82,0|H,11,0.9696176,2,109.20981429,1,162.70354241,0|C,11,1.50925462,2, 111.99245806,1,41.61016292,0 | H,14,0.96983329,11,109.3762261,2,66.31398 726,0 | H,14,0.96959808,11,109.33332679,2,-175.6059473,0 | N,14,1.46398122 ,11,111.31435947,2,-54.66821073,0 | C,17,1.46335303,14,110.92203212,11,-78.12363553,0 | H,18,0.95978569,17,109.47279196,14,-59.50551931,0 | H,18,0 .95977981,17,109.48180392,14,-179.5416663,0|H,18,0.96029005,17,109.479 41809,14,60.4817955,0 | C,17,1.46103942,14,110.03453426,11,160.73506063, 0 | H, 22, 0.96015783, 17, 109.50441192, 14, -59.75591802, 0 | H, 22, 0.96025804, 17 ,109.43504784,14,-179.75520143,0 | H,22,0.96009042,17,109.48244101,14,60 .25755645,0|C,1,2.61220359,2,145.38023704,7,-28.28046821,0|C,26,1.4214 094,1,61.86391641,2,45.90475752,0 | H,27,0.93001433,26,119.40330189,1,-1 15.26467384,0 | C,27,1.43412625,26,121.23354101,1,64.765803,0 | H,29,0.930 47733,27,120.21669104,26,164.86645894,0 | C,29,1.36284691,27,119.5281435 8,26,-15.13923495,0|H,31,0.92979605,29,120.36861049,27,-179.01672524,0 C, 31, 1.43623064, 29, 119.32220279, 27, 0.9750818, 0 H, 33, 0.92983777, 31, 119 .30084318,29,-166.30289302,0 Li,26,2.60978559,1,147.64074035,2,-179.47 265228,0 N,35,2.12270033,26,177.72086438,1,-7.5555009,0 C,36,1.4591408 3,35,106.58565173,26,157.51230206,0 | H,37,0.95995951,36,109.48429114,35 ,-68.73082123,0|H,37,0.95983992,36,109.46381677,35,51.24253335,0|H,37, 0.9599558,36,109.46704578,35,171.28793955,0 C,36,1.45682816,35,116.246 3274,26,35.39608153,0 | H,41,0.9598988,36,109.50801728,35,-178.57681344, 0|H,41,0.95989617,36,109.51096754,35,-58.49938321,0|H,41,0.96072409,36 ,109.47331879,35,61.4626441,0 C,36,1.46888952,35,103.84433854,26,-85.3 6957467,0|H,45,0.97026537,36,109.20627609,35,79.45559282,0|H,45,0.9696 176,36,109.20981429,35,-162.70354241,0 C,45,1.50925462,36,111.99245806 ,35,-41.61016292,0|H,48,0.96983329,45,109.3762261,36,-66.31398726,0|H, 48,0.96959808,45,109.33332679,36,175.6059473,0|N,48,1.46398122,45,111. 31435947,36,54.66821073,0 | C,51,1.46335303,48,110.92203212,45,78.123635 53,0 | H,52,0.95978569,51,109.47279196,48,59.50551931,0 | H,52,0.95977981, 51,109.48180392,48,179.5416663,0|H,52,0.96029005,51,109.47941809,48,-6 0.4817955,0 C,51,1.46103942,48,110.03453426,45,-160.73506063,0 H,56,0.

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96015783,51,109.50441192,48,59.75591802,0 |H,56,0.96025804,51,109.43504 784,48,179.75520143,0 |H,56,0.96009042,51,109.48244101,48,-60.25755645, 0 |C,33,1.41422489,31,121.45705094,29,13.72214156,0 |C,60,1.4214094,33,1 24.60599493,31,166.05829721,0 |H,61,0.93001433,60,119.40330189,33,-14.4 0677309,0 |C,61,1.43412625,60,121.23354101,33,165.56275007,0 |H,63,0.930 47733,61,120.21669104,60,-164.86645894,0 |C,63,1.36284691,61,119.528143 58,60,15.13923495,0 |H,65,0.92979605,63,120.36861049,61,179.01672524,0 | C,26,1.41422489,1,136.98418615,2,-65.86723645,0 |H,67,0.92983777,26,119 .24210122,1,98.16045561,0 || Version=IA32L-G03RevC.02 |State=1-AG|HF= -1088.4643129 |MP2=-1092.0511851 |RMSD=4.071e-009 |PG=CI [X(C22H40Li2N4)] | |@

2.8. MP2/6-311++G(d)

		_		Natural Pop	ulation	
Atom	No	Natural - Charge	Core	Valence	Rydberg	Total
Li	1	0.85740	1.99923	0.11352	0.02984	2.14260
N	2	-0.62353	1.99961	5.59724	0.02668	7.62353
С	3	-0.21726	1.99914	4.20327	0.01484	6.21726
Н	4	0.15723	0.00000	0.84137	0.00139	0.84277
Н	5	0.14618	0.0000	0.85293	0.00089	0.85382
Н	6	0.12817	0.00000	0.87069	0.00114	0.87183
С	7	-0.20751	1.99914	4.19405	0.01432	6.20751
Н	8	0.12517	0.00000	0.87380	0.00103	0.87483
Н	9	0.15115	0.00000	0.84794	0.00091	0.84885
Н	10	0.15481	0.00000	0.84423	0.00096	0.84519
С	11	-0.06829	1.99905	4.05162	0.01762	6.06829
H	12	0.14603	0.00000	0.85290	0.00107	0.85397
Н	13	0.13006	0.00000	0.86867	0.00127	0.86994
С	14	-0.06857	1.99907	4.05217	0.01733	6.06857
H	15	0.14101	0.00000	0.85797	0.00103	0.85899
Н	16	0.13431	0.00000	0.86450	0.00119	0.86569
N	17	-0.62734	1.99961	5.60452	0.02321	7.62734
С	18	-0.21855	1.99912	4.19934	0.02008	6.21855
Н	19	0.12445	0.00000	0.87441	0.00113	0.87555
Н	20	0.18228	0.00000	0.81624	0.00147	0.81772
Н	21	0.14337	0.0000	0.85571	0.00092	0.85663
С	22	-0.21056	1.99912	4.19714	0.01429	6.21056
Н	23	0.14160	0.0000	0.85772	0.00067	0.85840
Н	24	0.17590	0.0000	0.82316	0.00094	0.82410
Н	25	0.12287	0.0000	0.87619	0.00094	0.87713
С	26	0.02215	1.99916	3.94931	0.02937	5.97785
С	27	-0.51898	1.99917	4.47968	0.04012	6.51898
Н	28	0.14728	0.0000	0.85102	0.00170	0.85272
С	29	-0.23856	1.99929	4.20917	0.03010	6.23856
Н	30	0.13864	0.00000	0.86030	0.00106	0.86136
С	31	-0.25851	1.99931	4.22713	0.03208	6.25851
Н	32	0.14052	0.00000	0.85843	0.00104	0.85948
С	33	-0.48934	1.99889	4.44652	0.04394	6.48934
H	34	0.14494	0.00000	0.85334	0.00171	0.85506
Li	35	0.85878	1.99923	0.11353	0.02846	2.14122
N	36	-0.62340	1.99961	5.59726	0.02653	7.62340
С	37	-0.21724	1.99914	4.20326	0.01483	6.21724
Н	38	0.15724	0.0000	0.84137	0.00139	0.84276

-

Н	39	0.14619	0.00000	0.85293	0.00089	0.85381
Н	40	0.12817	0.00000	0.87069	0.00114	0.87183
С	41	-0.20751	1.99914	4.19405	0.01432	6.20751
Н	42	0.12517	0.00000	0.87380	0.00103	0.87483
	43	0 15115	0 00000	0 84794	0 00091	0 84885
и 11	10	0.15482	0.00000	0 84423	0 00095	0.84518
	15	0.13402	1 00005	4 05162	0.000000	0.04010
	45	-0.06629	1.99905	4.05163	0.01/01	0.00029
H	46	0.14603	0.00000	0.85290	0.00107	0.85397
Н	47	0.13006	0.00000	0.86867	0.00127	0.86994
C	48	-0.06856	1.99907	4.05217	0.01732	6.06856
H	49	0.14101	0.00000	0.85797	0.00103	0.85899
H	50	0.13431	0.00000	0.86450	0.00119	0.86569
N	51	-0.62730	1.99961	5.60450	0.02320	7.62730
С	52	-0.21851	1.99912	4.19935	0.02005	6.21851
Н	53	0.12445	0.00000	0.87441	0.00114	0.87555
Н	54	0.18229	0.00000	0.81625	0.00145	0.81771
Н	55	0.14337	0.00000	0.85570	0.00092	0.85663
С	56	-0.21055	1,99912	4.19714	0.01429	6.21055
н	57	0 14160	0 00000	0 85772	0 00067	0 85840
и И	58	0.17591	0 00000	0.82316	0 00093	0 82409
л ц	50	0.1007	0.00000	0.02510	0.00093	0.02400
п С	59	0.12207	1 00010	0.07019	0.00094	0.07713 E 00E07
C	60	0.01403	1.99918	3.95725	0.02954	5.98597
C	61	-0.51921	1.9991/	4.4/984	0.04019	6.51921
Н	62	0.14733	0.00000	0.85099	0.00168	0.85267
C	63	-0.23870	1.99929	4.20916	0.03025	6.23870
H	64	0.13867	0.00000	0.86029	0.00104	0.86133
С	65	-0.25392	1.99929	4.22296	0.03167	6.25392
Н	66	0.14055	0.00000	0.85844	0.00102	0.85945
С	67	-0.50592	1.99916	4.46310	0.04366	6.50592
Н	68	0.14658	0.00000	0.85181	0.00161	0.85342
======= * Tota	===== al *	0.00000	55.97813	======================================	======================================	206.00000
======= * Tota	===== al *	0.00000	55.97813	========== 149.27140	======================================	206.00000
======= * Tota	===== al *	0.00000	55.97813 Natur	======= 149.27140 al Populatio	======================================	206.00000
====== * Tota	===== al *	0.00000	55.97813 Natur	149.27140 al Populatio	========== 0.75046 n	206.00000
* Tota Core	===== al *	0.00000	55.97813 Natur 55.97813	======================================	========= 0.75046 n f 56)	206.00000
* Tota * Tota Core Valenc	===== al * 	0.00000	55.97813 Natur 55.97813 149.27140	149.27140 al Populatio 	======== 0.75046 n f 56) f 150)	206.00000
* Tota * Tota Core Valenc Natura	===== al * ce al Mi	0.00000	55.97813 Natur 55.97813 149.27140 205.24953	149.27140 al Populatio 	0.75046 n f 56) f 150) f 206)	206.00000
* Tota Core Valence Natura Natura	===== al * ce al Mi al Rv	0.00000 0.00000 nimal Basis dberg Basis	55.97813 Natur 55.97813 149.27140 205.24953 0.75046	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o	0.75046 n f 56) f 150) f 206) f 206)	206.00000
* Tota Core Valenc Natura Natura	al * ce al Mi al Ry	0.00000 0.00000 nimal Basis dberg Basis	55.97813 Natur 55.97813 149.27140 205.24953 0.75046	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o	0.75046 n f 56) f 150) f 206) f 206)	206.00000
* Tota Core Valenc Natura Natura	===== al * ce al Mi al Ry	0.00000 0.00000 nimal Basis dberg Basis	55.97813 Natur 55.97813 149.27140 205.24953 0.75046	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o	0.75046 n f 56) f 150) f 206) f 206)	206.00000
* Tota * Tota Core Valenc Natura Natura Atom	al * ce al Mi al Ry No	0.00000 nimal Basis dberg Basis	55.97813 Natur 55.97813 149.27140 205.24953 0.75046	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o 	0.75046 n f 56) f 150) f 206) f 206)	206.00000
* Tota Core Valenc Natura Natura Atom	al * ce al Mi al Ry No	0.00000 nimal Basis dberg Basis Natur	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 cal Electron	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati	0.75046 n f 56) f 150) f 206) f 206) on	206.00000
* Tota Core Valence Natura Natura Atom	2000	0.00000 nimal Basis dberg Basis Natur	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 ral Electron	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati	0.75046 n f 56) f 150) f 206) f 206) on	206.00000
* Tota Core Valence Natura Natura Atom	 al * al Mi al Ry No 	0.00000 nimal Basis dberg Basis Natur	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 cal Electron	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati	<pre></pre>	206.00000
* Tota Core Valence Natura Natura Atom	2000 2000 2000 2000 2000 2000	0.00000 nimal Basis dberg Basis Natur [core]2S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 cal Electron	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati	<pre> 0.75046 n f 56) f 150) f 206) f 206) on)) 4p(0.01)</pre>	206.00000
* Tota Core Valence Natura Natura Atom Li N C	2000 2000 2000	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Cal Electron (0.11)3d(0 (1.32)2p(4	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o 	<pre>0.75046 n f 56) f 150) f 206) f 206) on on))4p(0.01))4p(0.01)</pre>	206.00000
* Tota Core Valence Natura Natura Atom - Li N C H	200 x 200 x 20	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Cal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01	0.75046 n f 56) f 150) f 206) f 206) on on)) 4p(0.01)) 4p(0.01)	206.00000
* Tota Core Valence Natura Natura Atom - Li N C H H	200 x 200 x 20	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Tal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o 	0.75046 n f 56) f 150) f 206) f 206) on)) 4p(0.01)) 4p(0.01)	206.00000
* Tota * Tota Core Valence Natura Natura Atom - Li N C H H	===== al * ce al Mi al Ry NO 1 2 3 4 5 6	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S 1S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Tal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o 	0.75046 n f 56) f 150) f 206) f 206) on on)) 4p(0.01)) 4p(0.01)	206.00000
* Tota * Tota Core Valence Natura Natura Atom - Li N C H H H	===== al * ce al Mi al Ry NO 1 2 3 4 5 6 7	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S 1S 1S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Cal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (2.96)2p(2)2p(2)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01	<pre> 0.75046 n f 56) f 150) f 206) f 206) f 206) on)) 4p(0.01)) 4p(0.01)</pre>	206.00000
* Tota * Tota Core Valence Natura Natura Atom - Li N C H H H H C 	===== al * ce al Mi al Ry NO 1 2 3 4 5 6 7	0.00000 nimal Basis dberg Basis [core]2S [core]2S [core]2S [sore]2S [sore]2S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 ral Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.96)2p(3 (0.96)2p(3)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01	<pre> 0.75046 n f 56) f 150) f 206) f 206) f 206) on)) 4p(0.01)) 4p(0.01)) 4p(0.01)</pre>	206.00000
* Tota * Tota Core Valence Natura Natura Atom - Li N C H H H H H C H	===== al * ce al Mi al Ry No No 1 2 3 4 5 6 7 8 0	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S [sore]2S [sore]2S [sore]2S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 ral Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.96)2p(3 (0.87) (0.87)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01	<pre>0.75046 n f 56) f 150) f 206) f 206) f 206) on on))4p(0.01))4p(0.01))</pre>	206.00000
* Tota * Tota Core Valence Natura Natura Atom - Li N C H H H H H H H	al * 	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S [core]2S [so 1S [core]2S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Cal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.96)2p(3 (0.87) (0.85) (0.85) (0.85)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01	0.75046 n f 56) f 150) f 206) f 206) on)) 4p(0.01)) 4p(0.01))	206.00000
* Tota * Tota Core Valence Natura Natura Atom Li N C H H H H H H	===== al * ce al Mi al Ry No 1 2 3 4 5 6 7 8 9 10	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S [core]2S [sore]2S [sore]2S [sore]2S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Tal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.96)2p(3 (0.87) (0.85) (0.87) (0.85) (0.84)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati 	<pre>0.75046 n f 56) f 150) f 206) f 206) f 206) f 0.01)) 4p(0.01))</pre>	206.00000
* Tota * Tota Core Valence Natura Natura Atom Li N C H H H H H C H H H C	al * ce Al Mi Al Ry No No 1 2 3 4 5 6 7 8 9 10 11 1	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S [core]2S [sore]2S [sore]2S [sore]2S [sore]2S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Tal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.96)2p(3 (0.87) (0.96)2p(3 (0.87) (0.85) (0.84) (0.94)2p(3	<pre>149.27140 al Populatio</pre>	0.75046 n f 56) f 150) f 206) f 206) on)) 4p(0.01)) 4p(0.01)) 3d(0.01)	206.00000
* Tota * Tota Core Valence Natura Natura Atom - Li N C H H H H C H H H	al * al * al Mi al Ry No 1 2 3 4 5 6 7 8 9 10 11 12 2 3 4 5 6 7 8 9 10 11 12 10 10 10 10 10 10 10 10 10 10	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S [core]2S [s [core]2S [s [core]2S [s [s] 1S [s] 1S [s] 1S [s]	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Tal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.96)2p(3 (0.87) (0.96)2p(3 (0.87) (0.96)2p(3 (0.87) (0.85) (0.84) (0.94)2p(3 (0.85)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01 .24)3d(0.01 .12)3p(0.01	0.75046 n f 56) f 150) f 206) f 206) on)) 4p(0.01)) 4p(0.01)) 3d(0.01)	206.00000
* Tota * Tota Core Valence Natura Natura Atom - Li N C H H H H C H H H H H H H H H H	al * 	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S [core]2S [s] 1S [core]2S 1S 1S [core]2S 1S 1S 1S 1S 1S 1S 1S 1S 1S 1S 1S 1S 1S	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Tal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.85) (0.87) (0.85) (0.84) (0.94)2p(3 (0.85) (0.85) (0.87)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01 .24)3d(0.01 .12)3p(0.01	0.75046 n f 56) f 150) f 206) f 206) on)) 4p(0.01)) 4p(0.01)) 4p(0.01))	206.00000
* Tota Core Valence Natura Natura Atom - Li N C H H H H C H H H C H H H C H H H C H H H C H H H C	al * al * al Mi al Ry No 1 2 3 4 5 6 7 8 9 10 11 12 13 14	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S 1S 1S [core]2S 1S 1S [core]2S 1S 1S 1S 1S 1S 1S 1S 1S 1S 1	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Tal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.85) (0.87) (0.85) (0.84) (0.94)2p(3 (0.85) (0.87) (0.93)2p(3)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01 .12)3p(0.01 .12)3p(0.01	0.75046 n f 56) f 150) f 206) f 206) on)) 4p(0.01)) 4p(0.01)) 4p(0.01)) 3d(0.01)	206.00000
* Tota Core Valence Natura Natura Atom - Li N C H H H H C H H H C H H H C H H H C H H H C H H H C H H	al * al * al Mi al Ry No No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S 1S [core]2S 1S [core]2S 1S [core]2S 1S 1S [core]2S 1S 1S 1S 1S 1S 1S 1S 1S 1S 1	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Natur Cal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.85) (0.87) (0.85) (0.85) (0.84) (0.94)2p(3 (0.85) (0.87) (0.93)2p(3 (0.86)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01 .12)3p(0.01 .12)3p(0.01	0.75046 n f 56) f 150) f 206) f 206) on)) 4p(0.01)) 4p(0.01)) 4p(0.01)) 3d(0.01)	206.00000
* Tota Core Valence Natura Natura Atom - Li N C H H H H C H H H C H H H H C H H H H	al * al * ce al Mi al Ry No 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	0.00000 nimal Basis dberg Basis Natur [core]2S [core]2S [core]2S 1S [core]2S 1S [core]2S 1S [core]2S 1S 1S [core]2S 1S 1S 1S 1S 1S 1S 1S 1S 1S 1	55.97813 Natur 55.97813 149.27140 205.24953 0.75046 Tal Electron (0.11)3d(0 (1.32)2p(4 (0.96)2p(3 (0.84) (0.85) (0.87) (0.96)2p(3 (0.85) (0.87) (0.85) (0.84) (0.94)2p(3 (0.85) (0.85) (0.87) (0.93)2p(3 (0.86) (0.86)	149.27140 al Populatio (99.9609% o (99.5143% o (99.6357% o (0.3643% o Configurati .01)4p(0.02 .27)3p(0.01 .25)3d(0.01 .12)3p(0.01 .12)3p(0.01	0.75046 n f 56) f 150) f 206) f 206) on)) 4p(0.01)) 4p(0.01)) 4p(0.01)) 3d(0.01)) 3d(0.01)	206.00000

C H	18 19	[core]2S(1S(0.96)2p(0.87)	3.24)3d(0.01)	
н Н	20 21	1S (1S (0.82)			
С	22	[core]2S(0.96)2p(3.24)3d(0.01)	
Η	23	1S (0.86)			
Η	24	1S(0.82)			
H	25	1S(0.88)	2 22 2 1 (• • • • •
C	26	[core]2S(0.87)2p(3.08)3d(0.01)4p(0.02)
с u	27	[core]25(0.89)2p(3.59)4p(0.03)	
п С	20	[core]2S(0.03)	3 31)3d($0 \ 01)4p($	0 02)
H	30	[0010]25(1S(0.86)	5.51/5a(0.01/12(0.02/
С	31	[core]2S(0.91)2p(3.32)3d(0.01)4p(0.02)
Н	32	1S (0.86)		· _ ·	
С	33	[core]2S(0.87)2p(3.57)3p(0.01)4p(0.03)
Η	34	1S (0.85)			
Li	35	[core]2S(0.11)3d(0.01)4p(0.02)	
Ν	36	[core]2S(1.32)2p(4.27)3p(0.01)4p(0.01)
C	37	[core]2S(0.96)2p(3.25)3d(0.01)4p(0.01)
H	38	1S(1C(0.84)			
H	39	1S (0.85)			
н С	40	IS(0.87)	2 24)24(0 01)	
с н	41 42	[COIE]25(19(0.96)2p(5.24) SU(0.01)	
н	43	15(0.85)			
Н	44	1S (0.84)			
C	45	[core]2S(0.94)2p(3.12)3p(0.01)3d(0.01)
Н	46	1S (0.85)			
Н	47	1S(0.87)			
С	48	[core]2S(0.93)2p(3.12)3p(0.01)3d(0.01)
Η	49	1S (0.86)			
Η	50	1S(0.86)			
N	51	[core]2S(1.32)2p(4.28)4p(0.01)	
C	52	[core]2S(0.96)2p(3.24)3d(0.01)	
H	53	1S(0.87)			
п u	54	15(0.82)			
C	56	[core]2S(0.00)	3 24)3d(0 01)	
H	57	[0010]25(1S(0.86)	3.21/3a(0.017	
Н	58	1S (0.82)			
Н	59	1S (0.88)			
С	60	[core]2S(0.88)2p(3.08)3d(0.01)4p(0.02)
С	61	[core]2S(0.89)2p(3.59)4p(0.03)	
Η	62	1S (0.85)			
С	63	[core]2S(0.90)2p(3.31)3d(0.01)4p(0.02)
Η	64	1S(0.86)			
C	65	[core]2S(0.90)2p(3.32)3d(0.01)4p(0.02)
H	66	1S(U.86)		0 01 4 (0 02)
U TT	6/ 60	[core]2S(0.89)∠p(з.5/)зр(0.01)4p(0.03)
n	00	T2 (0.05/			

NBO analysis skipped by request.

1 |1 |UNPC-UNK|SP|RMP2-FC|6-311++G(d) |C22H40Li2N4|PCUSER|06-Sep-2008|0|| # MP2/6-311++G(D) POP=(NPA,FULL) GEOM=CONNECTIVITY SCF=TIGHT INT=ULTRA FINE||Single point on 2||0,1|Li|N,1,2.12270033|C,2,1.45914083,1,106. 58565173|H,3,0.95995951,2,109.48429114,1,68.73082123,0|H,3,0.95983992, 2,109.46381677,1,-51.24253335,0|H,3,0.9599558,2,109.46704578,1,-171.28 793955,0|C,2,1.45682816,1,116.2463274,3,122.11622054,0|H,7,0.9598988,2 ,109.50801728,1,178.57681344,0|H,7,0.95989617,2,109.51096754,1,58.4993

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8321,0 H.7,0.96072409,2,109.47331879,1,-61.4626441,0 C,2,1.46888952,1, 103.84433854,3,-117.11812327,0 | H,11,0.97026537,2,109.20627609,1,-79.45 559282,0|H,11,0.9696176,2,109.20981429,1,162.70354241,0|C,11,1.5092546 2,2,111.99245806,1,41.61016292,0|H,14,0.96983329,11,109.3762261,2,66.3 1398726,0|H,14,0.96959808,11,109.33332679,2,-175.6059473,0|N,14,1.4639 8122,11,111.31435947,2,-54.66821073,0 C,17,1.46335303,14,110.92203212, 11,-78.12363553,0|H,18,0.95978569,17,109.47279196,14,-59.50551931,0|H, 18,0.95977981,17,109.48180392,14,-179.5416663,0|H,18,0.96029005,17,109 .47941809,14,60.4817955,0 C,17,1.46103942,14,110.03453426,11,160.73506 063,0 | H,22,0.96015783,17,109.50441192,14,-59.75591802,0 | H,22,0.9602580 4,17,109.43504784,14,-179.75520143,0|H,22,0.96009042,17,109.48244101,1 4,60.25755645,0 | C,1,2.61220359,2,145.38023704,7,-28.28046821,0 | C,26,1. 4214094,1,61.86391641,2,45.90475752,0|H,27,0.93001433,26,119.40330189, 1,-115.26467384,0 | C,27,1.43412625,26,121.23354101,1,64.765803,0 | H,29,0 .93047733,27,120.21669104,26,164.86645894,0 C,29,1.36284691,27,119.528 14358,26,-15.13923495,0|H,31,0.92979605,29,120.36861049,27,-179.016725 24,0|C,31,1.43623064,29,119.32220279,27,0.9750818,0|H,33,0.92983777,31 ,119.30084318,29,-166.30289302,0 Li,26,2.60978559,1,147.64074035,2,-17 9.47265228,0 N,35,2.12270033,26,177.72086438,1,-7.5555009,0 C,36,1.459 14083,35,106.58565173,26,157.51230206,0|H,37,0.95995951,36,109.4842911 4,35,-68.73082123,0|H,37,0.95983992,36,109.46381677,35,51.24253335,0|H ,37,0.9599558,36,109.46704578,35,171.28793955,0C,36,1.45682816,35,116 .2463274,26,35.39608153,0 H,41,0.9598988,36,109.50801728,35,-178.57681 344,0 | H, 41,0.95989617,36,109.51096754,35,-58.49938321,0 | H, 41,0.9607240 9,36,109.47331879,35,61.4626441,0 C,36,1.46888952,35,103.84433854,26,-85.36957467,0|H,45,0.97026537,36,109.20627609,35,79.45559282,0|H,45,0. 9696176,36,109.20981429,35,-162.70354241,0|C,45,1.50925462,36,111.9924 5806,35,-41.61016292,0|H,48,0.96983329,45,109.3762261,36,-66.31398726, 0|H,48,0.96959808,45,109.33332679,36,175.6059473,0|N,48,1.46398122,45, 111.31435947,36,54.66821073,0 C,51,1.46335303,48,110.92203212,45,78.12 363553,0|H,52,0.95978569,51,109.47279196,48,59.50551931,0|H,52,0.95977 981, 51, 109.48180392, 48, 179.5416663, 0 H, 52, 0.96029005, 51, 109.47941809, 4 8,-60.4817955,0 C,51,1.46103942,48,110.03453426,45,-160.73506063,0 H,5 6,0.96015783,51,109.50441192,48,59.75591802,0|H,56,0.96025804,51,109.4 3504784,48,179.75520143,0 H,56,0.96009042,51,109.48244101,48,-60.25755 645,0 C,33,1.41422489,31,121.45705094,29,13.72214156,0 C,60,1.4214094, 33,124.60599493,31,166.05829721,0|H,61,0.93001433,60,119.40330189,33,-14.40677309,0 | C,61,1.43412625,60,121.23354101,33,165.56275007,0 | H,63,0 .93047733,61,120.21669104,60,-164.86645894,0 | C,63,1.36284691,61,119.52 814358,60,15.13923495,0|H,65,0.92979605,63,120.36861049,61,179.0167252 4,0 | C,26,1.41422489,1,136.98418615,2,-65.86723645,0 | H,67,0.92983777,26 ,119.24210122,1,98.16045561,0 || Version=IA32L-G03RevC.02 |State=1-AG |HF=-1088.6709503|MP2=-1092.4439169|RMSD=7.334e-009|PG=CI [X(C22H40Li2 N4)]||@

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