Supplementary Material (ESI) for Dalton Transactions

Structural Characterization and Bonding Properties of Lithium Naphthalene Radical Anion, $[Li^{+}(TMEDA)_2][C_{10}H_8^{\bullet -}]$, 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 ω=−34°) at values =0°, 120°, 240° with the detector at 2θ=−32°. For each of these runs, 606 frames were collected at 0.3° intervals and 30 s per frame. An additional run =0° of 100 frames was collected to improve redundancy. The diffraction frames were integrated using the program SAINT[1] 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_o^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_o>4σ(F_o). Structure **2** was solved by direct methods and refined to all 3261 unique F_o^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_o>4σ(F_o). 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**.

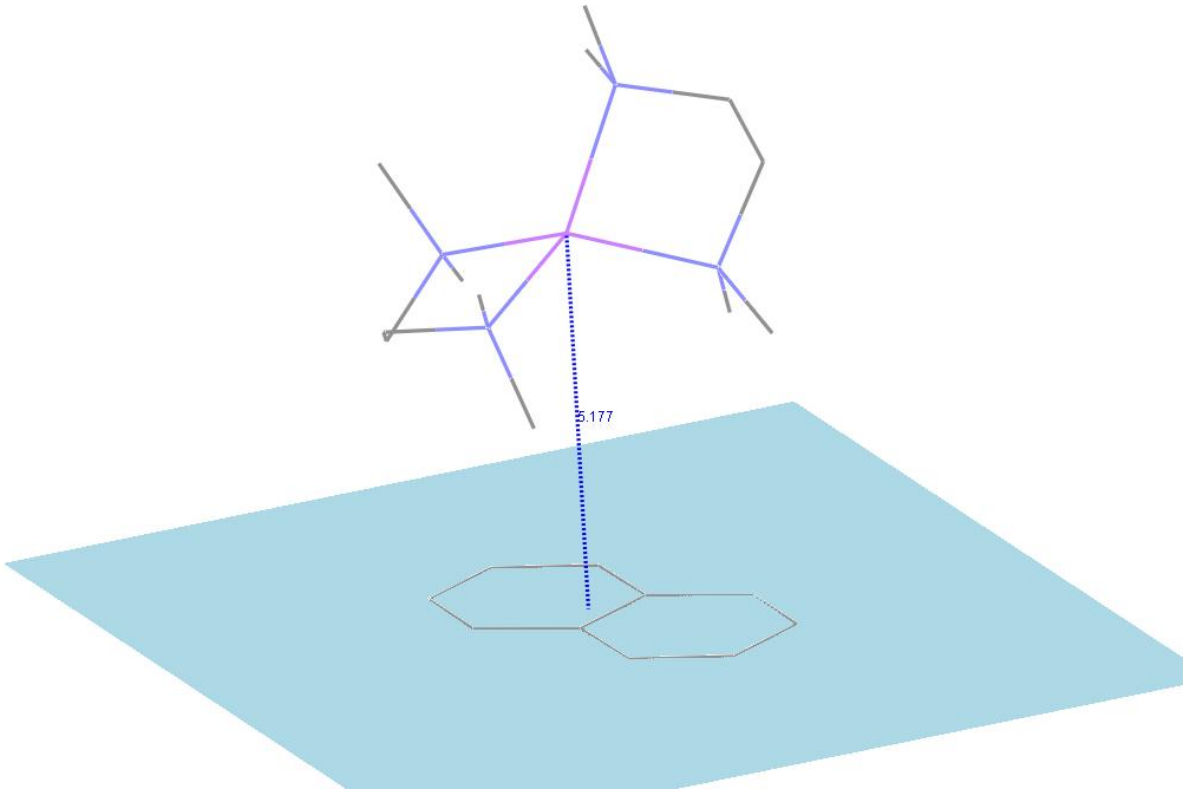

Figure S1. Calculated distance (5.18 ± 0.01 Å) between the lithium [$Li^{+}(TMEDA)_2$], and the least-squares mean plane of the anionic naphthalene moiety [$C_{10}H_8^{\bullet-}$] (blue plane), corresponding to **1**.

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. Comparison of structures: bond distances of **1**

Bond Distances for [Li+(TMEDA)2][C10H8•–] (**1**) (Angstroms)				Bond Distances for [K+(18-crown-6) (THF)2][C10H8•–] (ref. 5)		
Object 1	Object2	Length	e.s.d.	Length	e.s.d.	Absolute 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 differences:		0.00136

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

Table S2. Comparison of structures: bond distances of **1**

Bond Distances for [Li+(TMEDA)2][C10H8•–] (**1**) (Angstroms)				Bond Distances for [K+([2,2,2]-cryptand)][C10H8•–]		
Object 1	Object2	Length	e.s.d.	Length	e.s.d.	Absolute 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. Comparison of structures: bond angles of **1**

Bond angles for [Li+(TMEDA)2][C10H8•–] (**1**) (º)					Bond angles for [K+(18-crown-6) (THF)2][C10H8•–] (ref. 5) (º)		
Object1	Object2	Object3	Angle	e.s.d.	Angle	e.s.d.	Absolute 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	

Mean of absolute differences:	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. Comparison of structures: bond angles of **1**

Bond angles for [Li+(TMEDA)2][C10H8•–] (**1**) (º)					Bond angles for [K+([2,2,2]-cryptand)][C10H8•–] (ref. 5) (º)		
Object1	Object2	Object3	Angle	e.s.d.	Angle	e.s.d.	Absolute 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	

Mean of absolute differences:	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.

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

Bond distances for [(Li+TMEDA)2 C10H8–2] (**2**) (º)				Bond distances for [(Li+TMEDA)2 C10H8–2] (ref. 8) (º)		
Object1	Object2	Length	e.s.d.	Length	e.s.d.	Absolute difference
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
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

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. Comparison of structures: bond angles of **2**

Bond angles for [(Li+TMEDA)2 C10H8–2] (2) (°)					Bond angles for [(Li+TMEDA)2 C10H8–2] (ref. 8) (°)		
Object1	Object2	Object3	Angle	e.s.d.	Angle	e.s.d.	Absolute difference
N2	Li1	N1	85.24	0.08	85.2	0.4	0.05
C8	Li1	C9	36.27	0.05	36.7	0.2	0.43
C8	Li1	C11	73.77	0.07	73.3	0.3	0.47
C9	Li1	C10	34.60	0.05	34.5	0.3	0.1
C10	Li1	C11	36.41	0.05	36.1	0.3	0.31
C7	C8	C9	121.24	0.10	119.9	0.5	1.34
C8	C9	C10	119.52	0.10	120	0.5	0.48
C9	C10	C11	119.32	0.10	119.9	0.5	0.58
C10	C11	C7	121.46	0.10	121.3	0.5	0.16
C11	C7	C7	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	

Mean of absolute differences:	0.786

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

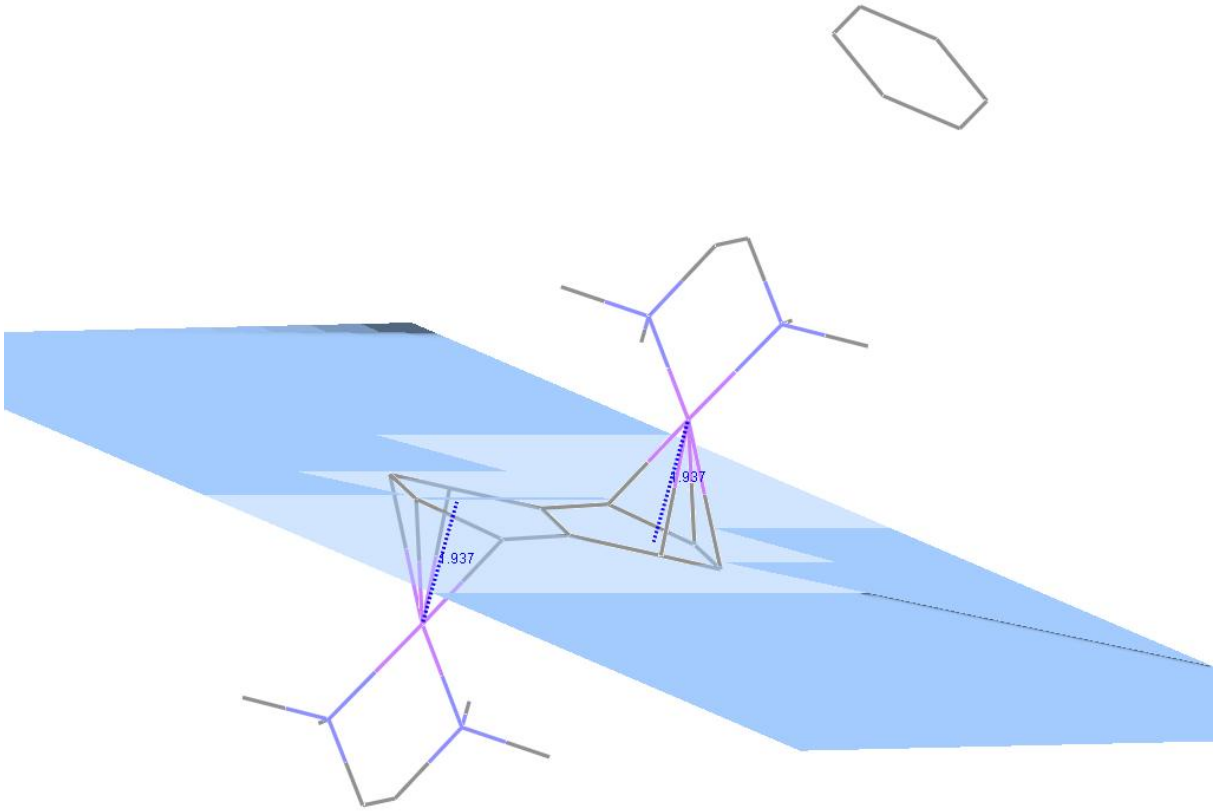

Figure S2. Calculated distance (1.937 ± 0.006 Å) between the lithium [Li^{+}(TMEDA)], and the least-squares mean plane of the anionic naphthalene moiety [$C_{10}H_8^{-2}$] (blue plane), corresponding to **2**.

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, DFT[5] using the B3LYP exchange-correlation functional,[6] and MP2[7] levels of theory were performed using the corresponding basis sets[8] 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)

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
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	1.99950	4.32667	0.01383	6.34000
H	4	0.20135	0.00000	0.79634	0.00231	0.79865
H	5	0.19029	0.00000	0.80827	0.00144	0.80971
H	6	0.17115	0.00000	0.82744	0.00141	0.82885
C	7	-0.33321	1.99951	4.32024	0.01346	6.33321
H	8	0.16810	0.00000	0.83056	0.00134	0.83190
H	9	0.19638	0.00000	0.80201	0.00161	0.80362
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	0.19842	0.00000	0.80009	0.00149	0.80158
H	13	0.18019	0.00000	0.81835	0.00146	0.81981
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	0.83156	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	0.04078	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	0.79634	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	0.80009	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	53	0.16705	0.00000	0.83156	0.00139	0.83295
H	54	0.22421	0.00000	0.77408	0.00171	0.77579
H	55	0.18694	0.00000	0.81167	0.00139	0.81306
C	56	-0.33462	1.99949	4.32166	0.01348	6.33462
H	57	0.18673	0.00000	0.81202	0.00125	0.81327
H	58	0.21893	0.00000	0.77927	0.00180	0.78107
H	59	0.16574	0.00000	0.83295	0.00131	0.83426
C	60	0.01895	1.99909	3.95395	0.02801	5.98105
C	61	-0.56242	1.99926	4.52237	0.04078	6.56242
H	62	0.18940	0.00000	0.80874	0.00186	0.81060
C	63	-0.28716	1.99931	4.25542	0.03244	6.28716
H	64	0.18130	0.00000	0.81693	0.00177	0.81870
C	65	-0.30196	1.99932	4.26986	0.03278	6.30196
H	66	0.18278	0.00000	0.81548	0.00175	0.81722
C	67	-0.54347	1.99925	4.50576	0.03847	6.54347
H	68	0.18806	0.00000	0.81002	0.00192	0.81194
* Total *		0.00000	55.98277	149.27873	0.73851	206.00000

Natural Population

Core	55.98277	(99.9692% of 56)
Valence	149.27873	(99.5192% of 150)
Natural Minimal Basis	205.26149	(99.6415% of 206)
Natural Rydberg Basis	0.73851	(0.3585% of 206)

Atom	No	Natural Electron Configuration
Li	1	[core]2S(0.08)3d(0.01)4p(0.01)
N	2	[core]2S(1.32)2p(4.30)3d(0.01)4p(0.02)
C	3	[core]2S(1.01)2p(3.32)3d(0.01)4p(0.01)
H	4	1S(0.80)
H	5	1S(0.81)
H	6	1S(0.83)
C	7	[core]2S(1.01)2p(3.31)3d(0.01)4p(0.01)
H	8	1S(0.83)
H	9	1S(0.80)
H	10	1S(0.80)
C	11	[core]2S(0.97)2p(3.18)3d(0.01)4p(0.01)
H	12	1S(0.80)
H	13	1S(0.82)
C	14	[core]2S(0.97)2p(3.18)3d(0.01)4p(0.01)
H	15	1S(0.81)
H	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	1S(0.77)
H	21	1S(0.81)
C	22	[core]2S(1.01)2p(3.31)3d(0.01)4p(0.01)
H	23	1S(0.81)
H	24	1S(0.78)
H	25	1S(0.83)
C	26	[core]2S(0.88)2p(3.07)3p(0.01)3d(0.01)4p(0.01)
C	27	[core]2S(0.92)2p(3.61)4p(0.03)
H	28	1S(0.81)
C	29	[core]2S(0.93)2p(3.33)4p(0.02)
H	30	1S(0.82)
C	31	[core]2S(0.93)2p(3.34)4p(0.02)

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

.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)

Summary of Natural Population Analysis:

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

H	20	0.18445	0.00000	0.81378	0.00177	0.81555
H	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
H	24	0.17783	0.00000	0.82058	0.00159	0.82217
H	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	0.00000	0.84760	0.00238	0.84998
C	29	-0.24112	1.99929	4.21219	0.02964	6.24112
H	30	0.14081	0.00000	0.85722	0.00197	0.85919
C	31	-0.25630	1.99929	4.22593	0.03109	6.25630
H	32	0.14273	0.00000	0.85537	0.00190	0.85727
C	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	0.00000	0.83860	0.00207	0.84067
H	39	0.14843	0.00000	0.84998	0.00160	0.85157
H	40	0.13026	0.00000	0.86793	0.00181	0.86974
C	41	-0.21550	1.99913	4.20348	0.01288	6.21550
H	42	0.12718	0.00000	0.87112	0.00171	0.87282
H	43	0.15347	0.00000	0.84495	0.00157	0.84653
H	44	0.15711	0.00000	0.84127	0.00163	0.84289
C	45	-0.07133	1.99905	4.05580	0.01648	6.07133
H	46	0.14758	0.00000	0.85060	0.00182	0.85242
H	47	0.13136	0.00000	0.86659	0.00205	0.86864
C	48	-0.07164	1.99906	4.05637	0.01621	6.07164
H	49	0.14255	0.00000	0.85567	0.00179	0.85745
H	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
H	53	0.12689	0.00000	0.87170	0.00141	0.87311
H	54	0.18443	0.00000	0.81377	0.00180	0.81557
H	55	0.14587	0.00000	0.85281	0.00133	0.85413
C	56	-0.21811	1.99912	4.20614	0.01285	6.21811
H	57	0.14395	0.00000	0.85472	0.00133	0.85605
H	58	0.17782	0.00000	0.82058	0.00160	0.82218
H	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
H	62	0.14998	0.00000	0.84763	0.00239	0.85002
C	63	-0.24101	1.99929	4.21222	0.02949	6.24101
H	64	0.14079	0.00000	0.85722	0.00199	0.85921
C	65	-0.26095	1.99931	4.23014	0.03150	6.26095
H	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
* Total *		0.00000	55.97805	149.26328	0.75867	206.00000

Natural Population

Core	55.97805	(99.9608% of 56)
Valence	149.26328	(99.5089% of 150)
Natural Minimal Basis	205.24133	(99.6317% of 206)
Natural Rydberg Basis	0.75867	(0.3683% of 206)

Atom	No	Natural Electron Configuration

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     Li    1      [core]2S( 0.11)3d( 0.01)4p( 0.01)
      N    2      [core]2S( 1.32)2p( 4.27)3p( 0.01)4p( 0.01)
      C    3      [core]2S( 0.96)2p( 3.25)3d( 0.01)
      H    4            1S( 0.84)
      H    5            1S( 0.85)
      H    6            1S( 0.87)
      C    7      [core]2S( 0.96)2p( 3.25)3d( 0.01)
      H    8            1S( 0.87)
      H    9            1S( 0.84)
      H   10            1S( 0.84)
      C   11      [core]2S( 0.94)2p( 3.12)3p( 0.01)3d( 0.01)
      H   12            1S( 0.85)
      H   13            1S( 0.87)
      C   14      [core]2S( 0.93)2p( 3.12)3p( 0.01)3d( 0.01)
      H   15            1S( 0.86)
      H   16            1S( 0.86)
      N   17      [core]2S( 1.32)2p( 4.28)4p( 0.01)
      C   18      [core]2S( 0.96)2p( 3.25)3d( 0.01)
      H   19            1S( 0.87)
      H   20            1S( 0.81)
      H   21            1S( 0.85)
      C   22      [core]2S( 0.96)2p( 3.25)3d( 0.01)
      H   23            1S( 0.85)
      H   24            1S( 0.82)
      H   25            1S( 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)
      H   28            1S( 0.85)
      C   29      [core]2S( 0.90)2p( 3.31)3d( 0.01)4p( 0.02)
      H   30            1S( 0.86)
      C   31      [core]2S( 0.90)2p( 3.32)3d( 0.01)4p( 0.02)
      H   32            1S( 0.86)
      C   33      [core]2S( 0.89)2p( 3.58)3p( 0.01)4p( 0.03)
      H   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)
      C   37      [core]2S( 0.96)2p( 3.25)3d( 0.01)
      H   38            1S( 0.84)
      H   39            1S( 0.85)
      H   40            1S( 0.87)
      C   41      [core]2S( 0.96)2p( 3.25)3d( 0.01)
      H   42            1S( 0.87)
      H   43            1S( 0.84)
      H   44            1S( 0.84)
      C   45      [core]2S( 0.94)2p( 3.12)3p( 0.01)3d( 0.01)
      H   46            1S( 0.85)
      H   47            1S( 0.87)
      C   48      [core]2S( 0.93)2p( 3.12)3p( 0.01)3d( 0.01)
      H   49            1S( 0.86)
      H   50            1S( 0.86)
      N   51      [core]2S( 1.32)2p( 4.28)4p( 0.01)
      C   52      [core]2S( 0.96)2p( 3.25)3d( 0.01)
      H   53            1S( 0.87)
      H   54            1S( 0.81)
      H   55            1S( 0.85)
      C   56      [core]2S( 0.96)2p( 3.25)3d( 0.01)
      H   57            1S( 0.85)
      H   58            1S( 0.82)
      H   59            1S( 0.87)
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      C   60      [core]2S( 0.87)2p( 3.07)3d( 0.01)4p( 0.02)
      C   61      [core]2S( 0.89)2p( 3.59)4p( 0.03)
      H   62           1S( 0.85)
      C   63      [core]2S( 0.90)2p( 3.31)3p( 0.01)3d( 0.01)4p( 0.01)
      H   64           1S( 0.86)
      C   65      [core]2S( 0.91)2p( 3.32)4p( 0.02)
      H   66           1S( 0.86)
      C   67      [core]2S( 0.87)2p( 3.58)3p( 0.01)4p( 0.03)
      H   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)

Summary of Natural Population Analysis:

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

H	47	0.20033	0.00000	0.79757	0.00210	0.79967
C	48	-0.22788	1.99934	4.21522	0.01332	6.22788
H	49	0.21334	0.00000	0.78524	0.00142	0.78666
H	50	0.20375	0.00000	0.79407	0.00218	0.79625
N	51	-0.59565	1.99960	5.57290	0.02315	7.59565
C	52	-0.41732	1.99943	4.40687	0.01102	6.41732
H	53	0.18652	0.00000	0.81164	0.00184	0.81348
H	54	0.24309	0.00000	0.75539	0.00151	0.75691
H	55	0.20759	0.00000	0.79115	0.00126	0.79241
C	56	-0.41347	1.99944	4.40326	0.01077	6.41347
H	57	0.20802	0.00000	0.79083	0.00114	0.79198
H	58	0.23663	0.00000	0.76146	0.00191	0.76337
H	59	0.18538	0.00000	0.81298	0.00164	0.81462
C	60	-0.04688	1.99910	4.02500	0.02278	6.04688
C	61	-0.54599	1.99930	4.49961	0.04708	6.54599
H	62	0.19673	0.00000	0.80063	0.00264	0.80327
C	63	-0.20676	1.99932	4.19117	0.01627	6.20676
H	64	0.17484	0.00000	0.82030	0.00486	0.82516
C	65	-0.37073	1.99939	4.33025	0.04109	6.37073
H	66	0.19487	0.00000	0.80282	0.00232	0.80513
C	67	-0.49270	1.99923	4.46514	0.02834	6.49270
H	68	0.19606	0.00000	0.80154	0.00240	0.80394
* Total *		0.01850	55.98166	149.33387	0.66597	205.98150

Natural Population

Core	55.98166	(99.9673% of 56)
Valence	149.33387	(99.5559% of 150)
Natural Minimal Basis	205.31553	(99.6677% of 206)
Natural Rydberg Basis	0.66597	(0.3233% of 206)

Atom	No	Natural Electron Configuration
Li	1	[core]2S(0.09)3d(0.01)4p(0.01)
N	2	[core]2S(1.31)2p(4.25)4p(0.01)
C	3	[core]2S(1.01)2p(3.40)4p(0.01)
H	4	1S(0.78)
H	5	1S(0.79)
H	6	1S(0.81)
C	7	[core]2S(1.01)2p(3.39)4p(0.01)
H	8	1S(0.81)
H	9	1S(0.78)
H	10	1S(0.78)
C	11	[core]2S(0.97)2p(3.24)4p(0.01)
H	12	1S(0.78)
H	13	1S(0.80)
C	14	[core]2S(0.97)2p(3.24)4p(0.01)
H	15	1S(0.79)
H	16	1S(0.79)
N	17	[core]2S(1.32)2p(4.26)4p(0.01)
C	18	[core]2S(1.01)2p(3.39)4p(0.01)
H	19	1S(0.81)
H	20	1S(0.76)
H	21	1S(0.79)
C	22	[core]2S(1.01)2p(3.39)4p(0.01)
H	23	1S(0.79)
H	24	1S(0.76)
H	25	1S(0.81)

```
      C   26      [core]2S( 0.88)2p( 3.14)3p( 0.01)4p( 0.01)
      C   27      [core]2S( 0.92)2p( 3.56)4p( 0.03)
      H   28            1S( 0.80)
      C   29      [core]2S( 0.93)2p( 3.37)4p( 0.02)
      H   30            1S( 0.80)
      C   31      [core]2S( 0.93)2p( 3.38)4p( 0.02)
      H   32            1S( 0.80)
      C   33      [core]2S( 0.92)2p( 3.55)4p( 0.02)
      H   34            1S( 0.80)
     Li   35      [core]2S( 0.09)3d( 0.01)4p( 0.01)
      N   36      [core]2S( 1.31)2p( 4.25)4p( 0.01)
      C   37      [core]2S( 1.01)2p( 3.40)4p( 0.01)
      H   38            1S( 0.78)
      H   39            1S( 0.79)
      H   40            1S( 0.81)
      C   41      [core]2S( 1.01)2p( 3.39)4p( 0.01)
      H   42            1S( 0.81)
      H   43            1S( 0.78)
      H   44            1S( 0.78)
      C   45      [core]2S( 0.97)2p( 3.24)4p( 0.01)
      H   46            1S( 0.78)
      H   47            1S( 0.80)
      C   48      [core]2S( 0.97)2p( 3.24)4p( 0.01)
      H   49            1S( 0.79)
      H   50            1S( 0.79)
      N   51      [core]2S( 1.32)2p( 4.26)4p( 0.01)
      C   52      [core]2S( 1.01)2p( 3.39)4p( 0.01)
      H   53            1S( 0.81)
      H   54            1S( 0.76)
      H   55            1S( 0.79)
      C   56      [core]2S( 1.01)2p( 3.39)4p( 0.01)
      H   57            1S( 0.79)
      H   58            1S( 0.76)
      H   59            1S( 0.81)
      C   60      [core]2S( 0.88)2p( 3.15)3p( 0.01)4p( 0.01)
      C   61      [core]2S( 0.92)2p( 3.58)4p( 0.04)
      H   62            1S( 0.80)
      C   63      [core]2S( 0.93)2p( 3.26)3p( 0.01)
      H   64            1S( 0.82)
      C   65      [core]2S( 0.93)2p( 3.40)4p( 0.03)
      H   66            1S( 0.80)
      C   67      [core]2S( 0.92)2p( 3.55)4p( 0.02)
      H   68            1S( 0.80)
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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
667739,0|H,18,0.95978967,17,109.48126841,14,-179.5447939,0|H,18,0.9603
```

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)

Summary of Natural Population Analysis:

			Natural Population			
Atom	No	Natural 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
C	3	-0.31998	1.99900	4.30984	0.01114	6.31998
H	4	0.18643	0.00000	0.81137	0.00219	0.81357
H	5	0.17547	0.00000	0.82293	0.00160	0.82453
H	6	0.15638	0.00000	0.84152	0.00210	0.84362
C	7	-0.31048	1.99900	4.30104	0.01044	6.31048
H	8	0.15351	0.00000	0.84461	0.00188	0.84649
H	9	0.18040	0.00000	0.81797	0.00162	0.81960
H	10	0.18436	0.00000	0.81388	0.00176	0.81564
C	11	-0.14146	1.99892	4.12847	0.01407	6.14146
H	12	0.17505	0.00000	0.82306	0.00190	0.82495
H	13	0.15942	0.00000	0.83831	0.00227	0.84058

C	14	-0.14183	1.99893	4.12908	0.01381	6.14183
H	15	0.17043	0.00000	0.82768	0.00188	0.82957
H	16	0.16340	0.00000	0.83436	0.00224	0.83660
N	17	-0.57758	1.99956	5.55441	0.02361	7.57758
C	18	-0.31925	1.99898	4.30966	0.01060	6.31925
H	19	0.15279	0.00000	0.84518	0.00204	0.84721
H	20	0.20923	0.00000	0.78856	0.00220	0.79077
H	21	0.17241	0.00000	0.82604	0.00156	0.82759
C	22	-0.31297	1.99898	4.30361	0.01038	6.31297
H	23	0.17184	0.00000	0.82684	0.00132	0.82816
H	24	0.20281	0.00000	0.79556	0.00163	0.79719
H	25	0.15182	0.00000	0.84643	0.00175	0.84818
C	26	-0.04932	1.99910	4.02722	0.02299	6.04932
C	27	-0.48247	1.99908	4.44576	0.03764	6.48247
H	28	0.16119	0.00000	0.83628	0.00252	0.83881
C	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
H	32	0.15931	0.00000	0.83866	0.00203	0.84069
C	33	-0.46236	1.99907	4.42930	0.03399	6.46236
H	34	0.16039	0.00000	0.83693	0.00268	0.83961
Li	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
H	38	0.18643	0.00000	0.81138	0.00220	0.81357
H	39	0.17547	0.00000	0.82293	0.00160	0.82453
H	40	0.15638	0.00000	0.84152	0.00210	0.84362
C	41	-0.31048	1.99900	4.30105	0.01044	6.31048
H	42	0.15351	0.00000	0.84461	0.00188	0.84649
H	43	0.18040	0.00000	0.81797	0.00162	0.81960
H	44	0.18436	0.00000	0.81388	0.00176	0.81564
C	45	-0.14145	1.99892	4.12846	0.01408	6.14145
H	46	0.17504	0.00000	0.82306	0.00190	0.82496
H	47	0.15942	0.00000	0.83831	0.00227	0.84058
C	48	-0.14183	1.99893	4.12908	0.01382	6.14183
H	49	0.17043	0.00000	0.82768	0.00188	0.82957
H	50	0.16340	0.00000	0.83436	0.00224	0.83660
N	51	-0.57762	1.99956	5.55444	0.02362	7.57762
C	52	-0.31927	1.99898	4.30965	0.01063	6.31927
H	53	0.15278	0.00000	0.84518	0.00204	0.84722
H	54	0.20921	0.00000	0.78856	0.00224	0.79079
H	55	0.17240	0.00000	0.82604	0.00156	0.82760
C	56	-0.31298	1.99898	4.30362	0.01038	6.31298
H	57	0.17184	0.00000	0.82684	0.00132	0.82816
H	58	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	4.44573	0.03763	6.48243
H	62	0.16116	0.00000	0.83632	0.00253	0.83884
C	63	-0.28022	1.99919	4.25729	0.02374	6.28022
H	64	0.15783	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
C	67	-0.44427	1.99879	4.41158	0.03390	6.44427
H	68	0.15850	0.00000	0.83861	0.00289	0.84150
* Total *		0.00000	55.97471	149.35068	0.67461	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)
 ---------------------------------------------------------

    Atom  No          Natural Electron Configuration
 ----------------------------------------------------------------------------
--
     Li    1      [core]2S( 0.12)3d( 0.01)4p( 0.02)5p( 0.01)
      N    2      [core]2S( 1.31)2p( 4.23)3p( 0.01)4p( 0.01)
      C    3      [core]2S( 0.97)2p( 3.34)3p( 0.01)
      H    4            1S( 0.81)
      H    5            1S( 0.82)
      H    6            1S( 0.84)
      C    7      [core]2S( 0.97)2p( 3.33)
      H    8            1S( 0.84)
      H    9            1S( 0.82)
      H   10            1S( 0.81)
      C   11      [core]2S( 0.94)2p( 3.19)3p( 0.01)
      H   12            1S( 0.82)
      H   13            1S( 0.84)
      C   14      [core]2S( 0.94)2p( 3.19)3p( 0.01)
      H   15            1S( 0.83)
      H   16            1S( 0.83)
      N   17      [core]2S( 1.32)2p( 4.24)4p( 0.01)
      C   18      [core]2S( 0.97)2p( 3.34)
      H   19            1S( 0.85)
      H   20            1S( 0.79)
      H   21            1S( 0.83)
      C   22      [core]2S( 0.97)2p( 3.34)
      H   23            1S( 0.83)
      H   24            1S( 0.80)
      H   25            1S( 0.85)
      C   26      [core]2S( 0.88)2p( 3.15)4p( 0.01)
      C   27      [core]2S( 0.90)2p( 3.55)4p( 0.03)
      H   28            1S( 0.84)
      C   29      [core]2S( 0.91)2p( 3.35)4p( 0.02)
      H   30            1S( 0.84)
      C   31      [core]2S( 0.91)2p( 3.36)4p( 0.02)
      H   32            1S( 0.84)
      C   33      [core]2S( 0.90)2p( 3.53)3p( 0.01)4p( 0.02)
      H   34            1S( 0.84)
     Li   35      [core]2S( 0.12)3d( 0.01)4p( 0.02)5p( 0.01)
      N   36      [core]2S( 1.31)2p( 4.23)3p( 0.01)4p( 0.01)
      C   37      [core]2S( 0.97)2p( 3.34)3p( 0.01)
      H   38            1S( 0.81)
      H   39            1S( 0.82)
      H   40            1S( 0.84)
      C   41      [core]2S( 0.97)2p( 3.33)
      H   42            1S( 0.84)
      H   43            1S( 0.82)
      H   44            1S( 0.81)
      C   45      [core]2S( 0.94)2p( 3.19)3p( 0.01)
      H   46            1S( 0.82)
      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)
```

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

Summary of Natural Population Analysis:

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

H	43	0.17657	0.00000	0.82219	0.00124	0.82343
H	44	0.18001	0.00000	0.81864	0.00134	0.81999
C	45	-0.12297	1.99919	4.10415	0.01963	6.12297
H	46	0.16831	0.00000	0.82968	0.00202	0.83169
H	47	0.14801	0.00000	0.84830	0.00370	0.85199
C	48	-0.12272	1.99920	4.10433	0.01919	6.12272
H	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
C	52	-0.29543	1.99925	4.28332	0.01286	6.29543
H	53	0.14086	0.00000	0.85619	0.00295	0.85914
H	54	0.20118	0.00000	0.79615	0.00267	0.79882
H	55	0.16702	0.00000	0.83177	0.00121	0.83298
C	56	-0.29005	1.99925	4.27888	0.01192	6.29005
H	57	0.16632	0.00000	0.83247	0.00122	0.83368
H	58	0.19855	0.00000	0.79974	0.00171	0.80145
H	59	0.13965	0.00000	0.85739	0.00296	0.86035
C	60	-0.00336	1.99914	3.97912	0.02510	6.00336
C	61	-0.52870	1.99919	4.48228	0.04723	6.52870
H	62	0.15761	0.00000	0.84073	0.00166	0.84239
C	63	-0.26241	1.99932	4.23420	0.02889	6.26241
H	64	0.14957	0.00000	0.84872	0.00172	0.85043
C	65	-0.27847	1.99932	4.24898	0.03017	6.27847
H	66	0.15108	0.00000	0.84727	0.00165	0.84892
C	67	-0.50281	1.99918	4.46158	0.04205	6.50281
H	68	0.15583	0.00000	0.84241	0.00176	0.84417
* Total *		0.00000	55.97872	149.30598	0.71530	206.00000

Natural Population

Core	55.97872	(99.9620% of 56)
Valence	149.30598	(99.5373% of 150)
Natural Minimal Basis	205.28470	(99.6528% of 206)
Natural Rydberg Basis	0.71530	(0.3472% of 206)

Atom	No	Natural Electron Configuration
Li	1	[core]2S(0.06)3p(0.02)
N	2	[core]2S(1.34)2p(4.22)3p(0.02)
C	3	[core]2S(0.98)2p(3.30)3p(0.01)
H	4	1S(0.82)
H	5	1S(0.83)
H	6	1S(0.85)
C	7	[core]2S(0.98)2p(3.30)3p(0.01)
H	8	1S(0.86)
H	9	1S(0.82)
H	10	1S(0.82)
C	11	[core]2S(0.96)2p(3.15)3p(0.02)
H	12	1S(0.83)
H	13	1S(0.85)
C	14	[core]2S(0.95)2p(3.15)3p(0.02)
H	15	1S(0.84)
H	16	1S(0.84)
N	17	[core]2S(1.35)2p(4.23)3p(0.02)
C	18	[core]2S(0.98)2p(3.30)3p(0.01)
H	19	1S(0.86)
H	20	1S(0.80)
H	21	1S(0.83)

```
      C   22      [core]2S( 0.98)2p( 3.30)3p( 0.01)
      H   23            1S( 0.83)
      H   24            1S( 0.80)
      H   25            1S( 0.86)
      C   26      [core]2S( 0.90)2p( 3.08)3p( 0.02)
      C   27      [core]2S( 0.92)2p( 3.56)3p( 0.05)
      H   28            1S( 0.84)
      C   29      [core]2S( 0.93)2p( 3.30)3p( 0.03)
      H   30            1S( 0.85)
      C   31      [core]2S( 0.93)2p( 3.31)3p( 0.03)
      H   32            1S( 0.85)
      C   33      [core]2S( 0.92)2p( 3.54)3p( 0.04)
      H   34            1S( 0.84)
     Li   35      [core]2S( 0.06)3p( 0.02)
      N   36      [core]2S( 1.34)2p( 4.22)3p( 0.02)
      C   37      [core]2S( 0.98)2p( 3.30)3p( 0.01)
      H   38            1S( 0.82)
      H   39            1S( 0.83)
      H   40            1S( 0.85)
      C   41      [core]2S( 0.98)2p( 3.30)3p( 0.01)
      H   42            1S( 0.86)
      H   43            1S( 0.82)
      H   44            1S( 0.82)
      C   45      [core]2S( 0.96)2p( 3.15)3p( 0.02)
      H   46            1S( 0.83)
      H   47            1S( 0.85)
      C   48      [core]2S( 0.95)2p( 3.15)3p( 0.02)
      H   49            1S( 0.84)
      H   50            1S( 0.84)
      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)
      H   55            1S( 0.83)
      C   56      [core]2S( 0.98)2p( 3.30)3p( 0.01)
      H   57            1S( 0.83)
      H   58            1S( 0.80)
      H   59            1S( 0.86)
      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            1S( 0.84)
      C   63      [core]2S( 0.93)2p( 3.30)3p( 0.03)
      H   64            1S( 0.85)
      C   65      [core]2S( 0.93)2p( 3.31)3p( 0.03)
      H   66            1S( 0.85)
      C   67      [core]2S( 0.92)2p( 3.54)3p( 0.04)
      H   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
```

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)

Summary of Natural Population Analysis:

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

C	11	-0.16092	1.99938	4.14386	0.01768	6.16092
H	12	0.19390	0.00000	0.80537	0.00073	0.80610
H	13	0.17582	0.00000	0.82348	0.00070	0.82418
C	14	-0.16005	1.99939	4.14323	0.01742	6.16005
H	15	0.18822	0.00000	0.81104	0.00075	0.81178
H	16	0.17943	0.00000	0.81983	0.00074	0.82057
N	17	-0.65631	1.99961	5.63187	0.02483	7.65631
C	18	-0.32121	1.99949	4.30706	0.01467	6.32121
H	19	0.16178	0.00000	0.83754	0.00068	0.83822
H	20	0.21885	0.00000	0.78019	0.00096	0.78115
H	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	0.00000	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
H	30	0.17570	0.00000	0.82341	0.00089	0.82430
C	31	-0.29622	1.99932	4.26378	0.03313	6.29622
H	32	0.17706	0.00000	0.82203	0.00091	0.82294
C	33	-0.53695	1.99925	4.49900	0.03870	6.53695
H	34	0.18233	0.00000	0.81661	0.00106	0.81767
Li	35	0.89105	1.99920	0.08367	0.02609	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
H	38	0.19581	0.00000	0.80257	0.00162	0.80419
H	39	0.18482	0.00000	0.81445	0.00074	0.81518
H	40	0.16578	0.00000	0.83352	0.00070	0.83422
C	41	-0.31593	1.99951	4.30195	0.01447	6.31593
H	42	0.16281	0.00000	0.83656	0.00063	0.83719
H	43	0.19091	0.00000	0.80819	0.00090	0.80909
H	44	0.19454	0.00000	0.80452	0.00094	0.80546
C	45	-0.16092	1.99938	4.14386	0.01768	6.16092
H	46	0.19390	0.00000	0.80537	0.00073	0.80610
H	47	0.17582	0.00000	0.82348	0.00070	0.82418
C	48	-0.16005	1.99939	4.14323	0.01742	6.16005
H	49	0.18822	0.00000	0.81104	0.00075	0.81178
H	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
H	54	0.21885	0.00000	0.78019	0.00096	0.78115
H	55	0.18159	0.00000	0.81773	0.00068	0.81841
C	56	-0.31768	1.99950	4.30367	0.01451	6.31768
H	57	0.18139	0.00000	0.81807	0.00053	0.81861
H	58	0.21339	0.00000	0.78555	0.00107	0.78661
H	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
C	63	-0.28151	1.99931	4.24943	0.03277	6.28151
H	64	0.17570	0.00000	0.82341	0.00089	0.82430
C	65	-0.29622	1.99932	4.26378	0.03313	6.29622
H	66	0.17706	0.00000	0.82203	0.00091	0.82294
C	67	-0.53695	1.99925	4.49900	0.03870	6.53695
H	68	0.18233	0.00000	0.81661	0.00106	0.81767
* Total *		0.00000	55.98283	149.29552	0.72165	206.00000

```
                                  Natural Population
 ---------------------------------------------------------------
   Core                      55.98283 ( 99.9693% of  56)
   Valence                  149.29552 ( 99.5303% of 150)
   Natural Minimal Basis    205.27835 ( 99.6497% of 206)
   Natural Rydberg Basis      0.72165 (  0.3503% of 206)
 ---------------------------------------------------------------

    Atom  No          Natural 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)
      C    3      [core]2S( 1.01)2p( 3.30)3d( 0.01)4p( 0.01)
      H    4            1S( 0.80)
      H    5            1S( 0.81)
      H    6            1S( 0.83)
      C    7      [core]2S( 1.01)2p( 3.30)3d( 0.01)4p( 0.01)
      H    8            1S( 0.84)
      H    9            1S( 0.81)
      H   10            1S( 0.80)
      C   11      [core]2S( 0.97)2p( 3.17)3d( 0.01)4p( 0.01)
      H   12            1S( 0.81)
      H   13            1S( 0.82)
      C   14      [core]2S( 0.97)2p( 3.18)3d( 0.01)4p( 0.01)
      H   15            1S( 0.81)
      H   16            1S( 0.82)
      N   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   19            1S( 0.84)
      H   20            1S( 0.78)
      H   21            1S( 0.82)
      C   22      [core]2S( 1.01)2p( 3.30)3d( 0.01)4p( 0.01)
      H   23            1S( 0.82)
      H   24            1S( 0.79)
      H   25            1S( 0.84)
      C   26      [core]2S( 0.88)2p( 3.07)3p( 0.01)3d( 0.01)4p( 0.01)
      C   27      [core]2S( 0.92)2p( 3.60)4p( 0.03)
      H   28            1S( 0.82)
      C   29      [core]2S( 0.92)2p( 3.32)3d( 0.01)4p( 0.02)
      H   30            1S( 0.82)
      C   31      [core]2S( 0.93)2p( 3.34)3d( 0.01)4p( 0.02)
      H   32            1S( 0.82)
      C   33      [core]2S( 0.91)2p( 3.59)4p( 0.03)
      H   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)
      C   37      [core]2S( 1.01)2p( 3.30)3d( 0.01)4p( 0.01)
      H   38            1S( 0.80)
      H   39            1S( 0.81)
      H   40            1S( 0.83)
      C   41      [core]2S( 1.01)2p( 3.30)3d( 0.01)4p( 0.01)
      H   42            1S( 0.84)
      H   43            1S( 0.81)
      H   44            1S( 0.80)
      C   45      [core]2S( 0.97)2p( 3.17)3d( 0.01)4p( 0.01)
      H   46            1S( 0.81)
      H   47            1S( 0.82)
      C   48      [core]2S( 0.97)2p( 3.18)3d( 0.01)4p( 0.01)
      H   49            1S( 0.81)
      H   50            1S( 0.82)
```

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

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)

Summary of Natural Population Analysis:

			Natural Population			
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
C	3	-0.21726	1.99914	4.20327	0.01484	6.21726
H	4	0.15723	0.00000	0.84137	0.00139	0.84277
H	5	0.14618	0.00000	0.85293	0.00089	0.85382
H	6	0.12817	0.00000	0.87069	0.00114	0.87183
C	7	-0.20751	1.99914	4.19405	0.01432	6.20751
H	8	0.12517	0.00000	0.87380	0.00103	0.87483
H	9	0.15115	0.00000	0.84794	0.00091	0.84885
H	10	0.15481	0.00000	0.84423	0.00096	0.84519
C	11	-0.06829	1.99905	4.05162	0.01762	6.06829
H	12	0.14603	0.00000	0.85290	0.00107	0.85397
H	13	0.13006	0.00000	0.86867	0.00127	0.86994
C	14	-0.06857	1.99907	4.05217	0.01733	6.06857
H	15	0.14101	0.00000	0.85797	0.00103	0.85899
H	16	0.13431	0.00000	0.86450	0.00119	0.86569
N	17	-0.62734	1.99961	5.60452	0.02321	7.62734
C	18	-0.21855	1.99912	4.19934	0.02008	6.21855
H	19	0.12445	0.00000	0.87441	0.00113	0.87555
H	20	0.18228	0.00000	0.81624	0.00147	0.81772
H	21	0.14337	0.00000	0.85571	0.00092	0.85663
C	22	-0.21056	1.99912	4.19714	0.01429	6.21056
H	23	0.14160	0.00000	0.85772	0.00067	0.85840
H	24	0.17590	0.00000	0.82316	0.00094	0.82410
H	25	0.12287	0.00000	0.87619	0.00094	0.87713
C	26	0.02215	1.99916	3.94931	0.02937	5.97785
C	27	-0.51898	1.99917	4.47968	0.04012	6.51898
H	28	0.14728	0.00000	0.85102	0.00170	0.85272
C	29	-0.23856	1.99929	4.20917	0.03010	6.23856
H	30	0.13864	0.00000	0.86030	0.00106	0.86136
C	31	-0.25851	1.99931	4.22713	0.03208	6.25851
H	32	0.14052	0.00000	0.85843	0.00104	0.85948
C	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
C	37	-0.21724	1.99914	4.20326	0.01483	6.21724
H	38	0.15724	0.00000	0.84137	0.00139	0.84276

H	39	0.14619	0.00000	0.85293	0.00089	0.85381
H	40	0.12817	0.00000	0.87069	0.00114	0.87183
C	41	-0.20751	1.99914	4.19405	0.01432	6.20751
H	42	0.12517	0.00000	0.87380	0.00103	0.87483
H	43	0.15115	0.00000	0.84794	0.00091	0.84885
H	44	0.15482	0.00000	0.84423	0.00095	0.84518
C	45	-0.06829	1.99905	4.05163	0.01761	6.06829
H	46	0.14603	0.00000	0.85290	0.00107	0.85397
H	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
C	52	-0.21851	1.99912	4.19935	0.02005	6.21851
H	53	0.12445	0.00000	0.87441	0.00114	0.87555
H	54	0.18229	0.00000	0.81625	0.00145	0.81771
H	55	0.14337	0.00000	0.85570	0.00092	0.85663
C	56	-0.21055	1.99912	4.19714	0.01429	6.21055
H	57	0.14160	0.00000	0.85772	0.00067	0.85840
H	58	0.17591	0.00000	0.82316	0.00093	0.82409
H	59	0.12287	0.00000	0.87619	0.00094	0.87713
C	60	0.01403	1.99918	3.95725	0.02954	5.98597
C	61	-0.51921	1.99917	4.47984	0.04019	6.51921
H	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
C	65	-0.25392	1.99929	4.22296	0.03167	6.25392
H	66	0.14055	0.00000	0.85844	0.00102	0.85945
C	67	-0.50592	1.99916	4.46310	0.04366	6.50592
H	68	0.14658	0.00000	0.85181	0.00161	0.85342
* Total *		0.00000	55.97813	149.27140	0.75046	206.00000

Natural Population

Core	55.97813	(99.9609% of 56)
Valence	149.27140	(99.5143% of 150)
Natural Minimal Basis	205.24953	(99.6357% of 206)
Natural Rydberg Basis	0.75046	(0.3643% of 206)

Atom	No	Natural Electron Configuration
Li	1	[core]2S(0.11)3d(0.01)4p(0.02)
N	2	[core]2S(1.32)2p(4.27)3p(0.01)4p(0.01)
C	3	[core]2S(0.96)2p(3.25)3d(0.01)4p(0.01)
H	4	1S(0.84)
H	5	1S(0.85)
H	6	1S(0.87)
C	7	[core]2S(0.96)2p(3.24)3d(0.01)
H	8	1S(0.87)
H	9	1S(0.85)
H	10	1S(0.84)
C	11	[core]2S(0.94)2p(3.12)3p(0.01)3d(0.01)
H	12	1S(0.85)
H	13	1S(0.87)
C	14	[core]2S(0.93)2p(3.12)3p(0.01)3d(0.01)
H	15	1S(0.86)
H	16	1S(0.86)
N	17	[core]2S(1.32)2p(4.28)4p(0.01)

```
      C   18      [core]2S( 0.96)2p( 3.24)3d( 0.01)
      H   19            1S( 0.87)
      H   20            1S( 0.82)
      H   21            1S( 0.86)
      C   22      [core]2S( 0.96)2p( 3.24)3d( 0.01)
      H   23            1S( 0.86)
      H   24            1S( 0.82)
      H   25            1S( 0.88)
      C   26      [core]2S( 0.87)2p( 3.08)3d( 0.01)4p( 0.02)
      C   27      [core]2S( 0.89)2p( 3.59)4p( 0.03)
      H   28            1S( 0.85)
      C   29      [core]2S( 0.90)2p( 3.31)3d( 0.01)4p( 0.02)
      H   30            1S( 0.86)
      C   31      [core]2S( 0.91)2p( 3.32)3d( 0.01)4p( 0.02)
      H   32            1S( 0.86)
      C   33      [core]2S( 0.87)2p( 3.57)3p( 0.01)4p( 0.03)
      H   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)
      C   37      [core]2S( 0.96)2p( 3.25)3d( 0.01)4p( 0.01)
      H   38            1S( 0.84)
      H   39            1S( 0.85)
      H   40            1S( 0.87)
      C   41      [core]2S( 0.96)2p( 3.24)3d( 0.01)
      H   42            1S( 0.87)
      H   43            1S( 0.85)
      H   44            1S( 0.84)
      C   45      [core]2S( 0.94)2p( 3.12)3p( 0.01)3d( 0.01)
      H   46            1S( 0.85)
      H   47            1S( 0.87)
      C   48      [core]2S( 0.93)2p( 3.12)3p( 0.01)3d( 0.01)
      H   49            1S( 0.86)
      H   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)
      H   54            1S( 0.82)
      H   55            1S( 0.86)
      C   56      [core]2S( 0.96)2p( 3.24)3d( 0.01)
      H   57            1S( 0.86)
      H   58            1S( 0.82)
      H   59            1S( 0.88)
      C   60      [core]2S( 0.88)2p( 3.08)3d( 0.01)4p( 0.02)
      C   61      [core]2S( 0.89)2p( 3.59)4p( 0.03)
      H   62            1S( 0.85)
      C   63      [core]2S( 0.90)2p( 3.31)3d( 0.01)4p( 0.02)
      H   64            1S( 0.86)
      C   65      [core]2S( 0.90)2p( 3.32)3d( 0.01)4p( 0.02)
      H   66            1S( 0.86)
      C   67      [core]2S( 0.89)2p( 3.57)3p( 0.01)4p( 0.03)
      H   68            1S( 0.85)


 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
```

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
,37,0.9599558,36,109.46704578,35,171.28793955,0|C,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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