Supplementary material (ESI) for Journal of Materials Chemistry

The Synthesis and Structural Investigation of Mixed Lithium / Sodium Amides

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Supplementary Crystallographic Information for System II

x = 1

R_ expected	8.132	R_expected'	17.074
R_weighted pattern	17.815	R_weighted pattern'	37.408
R_Pattern	13.547	R_Pattern'	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name		LiNH2_00					
Space Group		I – 4					
Scale		0.000010(9)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.000182(2)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)

Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.000006(1)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_0 + 0.2*aLi_{10} = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000010(6)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_04
Space Group	I – 4
Scale	0.0000010(4)
Lattice Parameter	a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å
	c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å
Occupancy Parameter	oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)

Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000010(4)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_07
Space Group	I – 4
Scale	0.0000010(3)
Lattice Parameter	a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å

		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_10

Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000026(1)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.00000000(3)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000001(1)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å				
			c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_02				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_03
Space Group	I – 4

Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å				
			c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_04				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å				
			c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_05				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å				
			c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_06
Space Group	I – 4
Scale	0.0000001(2)
Lattice Parameter	a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å

			c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_07				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å				
			c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_08				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)				
			c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_09
Space Group	I – 4
Scale	0.0000001(2)
Lattice Parameter	a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å
	c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å
Nitrogen Z Coordinate	z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)

Occupancy Parameter			oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_10				
Space Group			I – 4				
Scale			0.0000001(1)				
Lattice Parameter			a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å				
			c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.0000000(1)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

X = 0.917

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name		LiNH2_00					
Space Group		I – 4					
Scale		0.0000061(3)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.0000192(4)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000396(5)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)

Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000401(5)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000324(5)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000235(4)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-	0.02(1)	b_{eq}= 0.1(3)

					oLi05)		
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000108(3)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000042(3)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000023(2)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)

Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000011(2)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_10					
Space Group		I – 4					
Scale		0.0000028(2)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000041(1)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148

Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.00000055(3)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000025(1)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_01
Space Group	I – 4
Scale	0.0000049(4)
Lattice Parameter	a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å
	c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å
Nitrogen Z Coordinate	z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)

Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_02				
Space Group			I – 4				
Scale			0.0000087(5)				
Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_03				
Space Group			I – 4				
Scale			0.0000099(5)				
Lattice Parameter			a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å				
			c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_04				
Space Group			I – 4				
Scale			0.0000095(5)				
Lattice Parameter			a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å				
			c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484

Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_05					
Space Group		I – 4					
Scale		0.0000109(5)					
Lattice Parameter		a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å					
		c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)					
Occupancy Parameter		oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_06					
Space Group		I – 4					
Scale		0.0000089(5)					
Lattice Parameter		a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å					
		c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)					
Occupancy Parameter		oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_07					
Space Group		I – 4					
Scale		0.0000072(5)					
Lattice Parameter		a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å					
		c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)					
Occupancy Parameter		oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484

Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_08					
Space Group		I – 4					
Scale		0.0000067(4)					
Lattice Parameter		$a = b = a\_08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)$					
		$c = c_08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.2*z\_N_0 + 0.8*z\_N_{10} = 0.1012(6)$					
Occupancy Parameter		$oNa08 = 0.2*yNa_0 + 0.8*yNa_{10} = 0.79(2)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_09					
Space Group		I – 4					
Scale		0.0000021(3)					
Lattice Parameter		$a = b = a_09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)$Å					
		$c = c_09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.1*z\_N_0 + 0.9*z\_N_{10} = 0.1012(7)$					
Occupancy Parameter		$oNa09 = 0.1*yNa_0 + 0.9*yNa_{10} = 0.77(2)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_10					
Space Group		I – 4					
Scale		0.0000038(3)					
Lattice Parameter		$a = b = a_10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)$Å					
		$c = c_10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.0*z\_N_0 + 1.0*z\_N_{10} = 0.1012(8)$					
Occupancy Parameter		$oNa10 = 0.0*yNa_0 + 1.0*yNa_{10} = 0.75(2)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484

Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		NaNH2					
Space Group		Fddd					
Scale		0.000000011(7)					
Lattice Parameter		a = 8.95918(2) Å					
		b = 10.45229(3) Å					
		c = 8.07224(2) Å					
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.833

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name		LiNH2_00					
Space Group		I – 4					
Scale		0.0000028(3)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_01
Space Group	I – 4

Scale		0.0000073(5)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000134(6)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000129(6)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000103(6)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000075(5)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000035(4)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)

Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000011(4)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)

Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_10					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000037(1)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.00000280(6)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.000000(3)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.0000144(5)				
Lattice Parameter			a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å				
			c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_02				
Space Group			I – 4				
Scale			0.0000251(6)				
Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484

Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_03					
Space Group		I – 4					
Scale		0.0000196(5)					
Lattice Parameter		a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å					
		c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)					
Occupancy Parameter		oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_04					
Space Group		I – 4					
Scale		0.0000154(5)					
Lattice Parameter		a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å					
		c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)					
Occupancy Parameter		oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_05					
Space Group		I – 4					
Scale		0.0000128(5)					
Lattice Parameter		a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å					
		c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)					
Occupancy Parameter		oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484

Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_06					
Space Group		I – 4					
Scale		0.0000095(5)					
Lattice Parameter		a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å					
		c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)					
Occupancy Parameter		oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_07					
Space Group		I – 4					
Scale		0.0000071(4)					
Lattice Parameter		a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å					
		c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)					
Occupancy Parameter		oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_08					
Space Group		I – 4					
Scale		0.0000041(4)					
Lattice Parameter		a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)					
		c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)					
Occupancy Parameter		oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_09				
Space Group			I – 4				
Scale			0.0000023(3)				
Lattice Parameter			a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å				
			c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)				
Occupancy Parameter			oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_10				
Space Group			I – 4				
Scale			0.0000018(2)				
Lattice Parameter			a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å				
			c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.00000001(1)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.750

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		

Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name		LiNH2_00					
Space Group		I – 4					
Scale		0.0000017(3)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.0000034(5)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_02
Space Group	I – 4
Scale	0.0000060(5)
Lattice Parameter	a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å
	c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å

Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000040(5)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000040(4)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_05
Space Group	I – 4

Scale		0.0000024(4)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_10					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)

Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name			Li2O				
Space Group			Fm3m				
Scale			0.000045(2)				
Lattice Parameter			a = b = c = 4.6113(1) Å				
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name			LiNa2(NH2)3				
Space Group			P42/m				
Scale			0.0000105(1)				
Lattice Parameter			a = b = 6.28325(1)Å				
			c = 11.14942(2)Å				
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000001(5)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484

Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_01					
Space Group		I – 4					
Scale		0.0000658(9)					
Lattice Parameter		$a = b = a_01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)$Å					
		$c = c\_01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2)$ Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.9*\ z\_N_0 + 0.1*\ z\_N_{10} = 0.1012(3)$					
Occupancy Parameter		$oNa01 = 0.9*\ yNa_0 + 0.1*yNa_{10} = 0.939(7)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_02					
Space Group		I – 4					
Scale		0.0000386(7)					
Lattice Parameter		$a = b = a_02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)$Å					
		$c = c_02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.8*\ z\_N_0 + 0.2*\ z\_N_{10} = 0.1012(3)$					
Occupancy Parameter		$oNa02 = 0.8*\ yNa_0 + 0.2*yNa_{10} = 0.918(9)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_03					
Space Group		I – 4					
Scale		0.0000180(6)					
Lattice Parameter		$a = b = a_03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)$Å					
		$c = c_03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.7*\ z\_N_0 + 0.3*\ z\_N_{10} = 0.1012(4)$					
Occupancy Parameter		$oNa03 = 0.7*\ yNa_0 + 0.3*yNa_{10} = 0.90(1)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_04				
Space Group			I – 4				
Scale			0.0000110(5)				
Lattice Parameter			a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å				
			c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_05				
Space Group			I – 4				
Scale			0.0000086(5)				
Lattice Parameter			a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å				
			c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_06				
Space Group			I – 4				
Scale			0.0000056(5)				
Lattice Parameter			a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å				
			c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_07

Space Group			I – 4				
Scale			0.0000046(4)				
Lattice Parameter			a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å				
			c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_08				
Space Group			I – 4				
Scale			0.0000022(3)				
Lattice Parameter			a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)				
			c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_09				
Space Group			I – 4				
Scale			0.0000013(3)				
Lattice Parameter			a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å				
			c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)				
Occupancy Parameter			oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_10
Space Group	I – 4
Scale	0.0000007(2)

Lattice Parameter			a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å				
			c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.00000000(1)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.667

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name			LiNH2_00				
Space Group			I – 4				
Scale			0.0000010(2)				
Lattice Parameter			a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å				
			c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å				
Occupancy Parameter			oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)				
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)

Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_03
Space Group	I – 4
Scale	0.0000010(2)
Lattice Parameter	a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å
	c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å
Occupancy Parameter	oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)

Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_06
Space Group	I – 4
Scale	0.0000010(2)
Lattice Parameter	a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å

		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_09

Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_10					
Space Group		I – 4					
Scale		0.0000010(1)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000070(2)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.0000286(2)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810

Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000055(5)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.000079(1)				
Lattice Parameter			a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å				
			c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_02

Space Group			I – 4				
Scale			0.0000067(6)				
Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_03				
Space Group			I – 4				
Scale			0.0000029(4)				
Lattice Parameter			a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å				
			c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_04				
Space Group			I – 4				
Scale			0.0000013(3)				
Lattice Parameter			a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å				
			c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_05
Space Group	I – 4
Scale	0.0000007(3)

Lattice Parameter			a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å				
			c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_06				
Space Group			I – 4				
Scale			0.0000007(3)				
Lattice Parameter			a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å				
			c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_07				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å				
			c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_08
Space Group	I – 4
Scale	0.0000003(2)
Lattice Parameter	a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)
	c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å

Nitrogen Z Coordinate			z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_09				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å				
			c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)				
Occupancy Parameter			oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_10				
Space Group			I – 4				
Scale			0.0000002(2)				
Lattice Parameter			a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å				
			c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.00000000(1)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283

Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.583

R_ expected	8.132	R_expected'	17.074
R_weighted pattern	17.815	R_weighted pattern'	37.408
R_Pattern	13.547	R_Pattern'	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name		LiNH2_00					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.0000016(4)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)

Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000010(4)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_0 + 0.2*aLi_{10} = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ	0.98(1)	b_{eq}= 0.1(3)

					(oLi04)		
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_07
Space Group	I – 4
Scale	0.0000010(2)
Lattice Parameter	a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å
	c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å
Occupancy	oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)

Parameter							
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_10
Space Group	I – 4
Scale	0.0000010(2)

Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000044(2)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.0000431(2)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name	Li3Na(NH2)4_00
Space Group	I – 4

Scale			0.0000023(2)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.000087(1)				
Lattice Parameter			a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å				
			c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_02				
Space Group			I – 4				
Scale			0.0000140(7)				
Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_03
Space Group	I – 4
Scale	0.0000036(5)
Lattice Parameter	a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å

			c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_04				
Space Group			I – 4				
Scale			0.0000023(4)				
Lattice Parameter			a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0763(3) Å				
			c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_05				
Space Group			I – 4				
Scale			0.0000009(4)				
Lattice Parameter			a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å				
			c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_06
Space Group	I – 4
Scale	0.0000017(4)
Lattice Parameter	a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å
	c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å
Nitrogen Z Coordinate	z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)

Occupancy Parameter			oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_07				
Space Group			I – 4				
Scale			0.0000003(3)				
Lattice Parameter			a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å				
			c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_08				
Space Group			I – 4				
Scale			0.0000002(3)				
Lattice Parameter			a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)				
			c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_09				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å				
			c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)				
Occupancy Parameter			oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484

Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_10				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å				
			c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.00000008(1)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.5

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name		LiNH2_00					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)

Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-	0.02(1)	b_{eq}= 0.1(3)

					oLi05)		
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)

Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_10					
Space Group		I – 4					
Scale		0.0000010(1)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000034(1)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148

Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.0000421(2)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000023(4)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_01
Space Group	I – 4
Scale	0.0000386(7)
Lattice Parameter	a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å
	c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å
Nitrogen Z Coordinate	z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)

Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_02				
Space Group			I – 4				
Scale			0.0000034(5)				
Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_03				
Space Group			I – 4				
Scale			0.0000008(3)				
Lattice Parameter			a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å				
			c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_04				
Space Group			I – 4				
Scale			0.0000008(3)				
Lattice Parameter			a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å				
			c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484

Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_05					
Space Group		I – 4					
Scale		0.0000002(3)					
Lattice Parameter		a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å					
		c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)					
Occupancy Parameter		oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_06					
Space Group		I – 4					
Scale		0.0000001(2)					
Lattice Parameter		a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å					
		c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)					
Occupancy Parameter		oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_07					
Space Group		I – 4					
Scale		0.0000001(2)					
Lattice Parameter		a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å					
		c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)					
Occupancy Parameter		oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484

Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_08					
Space Group		I – 4					
Scale		0.0000001(2)					
Lattice Parameter		a = b = a_ 08 = $0.2*a_{10} + 0.8*a_{10}$ = 5.0696(2)					
		c = c_ 08 = $0.2*c_{10} + 0.8*c_{10}$ = 11.3436(6)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)					
Occupancy Parameter		oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_09					
Space Group		I – 4					
Scale		0.0000001(2)					
Lattice Parameter		a = b = a_ 09 = $0.1*a_{10} + 0.9*a_{10}$ = 5.0679(2)Å					
		c = c_ 09 = $0.1*c_{10} + 0.9*c_{10}$ = 11.3196(6)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)					
Occupancy Parameter		oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_10					
Space Group		I – 4					
Scale		0.0000001(2)					
Lattice Parameter		a = b = a_ 10 = $0.0*a_{10} + 1.0*a_{10}$ = 5.0662(2)Å					
		c = c_ 10 = $0.0*c_{10} + 1.0*c_{10}$ = 11.2957(7)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)					
Occupancy Parameter		oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484

Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		NaNH2					
Space Group		Fddd					
Scale		0.00000000(1)					
Lattice Parameter		a = 8.95918(2) Å					
		b = 10.45229(3) Å					
		c = 8.07224(2) Å					
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.417

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name		LiNH2_00					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_01
Space Group	I – 4

Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)

Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)

Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_10					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000065(2)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.0001002(3)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000008(3)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.0000133(5)				
Lattice Parameter			a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å				
			c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_02				
Space Group			I – 4				
Scale			0.0000022(4)				
Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484

Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_03					
Space Group		I – 4					
Scale		0.0000007(3)					
Lattice Parameter		a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å					
		c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)					
Occupancy Parameter		oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_04					
Space Group		I – 4					
Scale		0.0000002(3)					
Lattice Parameter		a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å					
		c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)					
Occupancy Parameter		oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_05					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å					
		c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)					
Occupancy Parameter		oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484

Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_06					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å					
		c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)					
Occupancy Parameter		oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_07					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å					
		c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)					
Occupancy Parameter		oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_08					
Space Group		I – 4					
Scale		0.0000001(2)					
Lattice Parameter		a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)					
		c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)					
Occupancy Parameter		oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_09				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å				
			c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)				
Occupancy Parameter			oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_10				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å				
			c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.00000000(1)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.333

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name		LiNH2_00					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_02
Space Group	I – 4
Scale	0.0000010(3)
Lattice Parameter	a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å
	c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å
Occupancy Parameter	oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)

Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_05
Space Group	I – 4
Scale	0.0000010(3)
Lattice Parameter	a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å

		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_08

Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_10					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)

Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000203(2)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.0001320(4)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.0000010(3)				
Lattice Parameter			a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å				
			c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_02				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_03				
Space Group			I – 4				
Scale			0.0000004(3)				
Lattice Parameter			a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å				
			c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_04

Space Group			I – 4				
Scale			0.0000005(3)				
Lattice Parameter			a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å				
			c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_05				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å				
			c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_06				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å				
			c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_07
Space Group	I – 4
Scale	0.0000003(3)

Lattice Parameter			a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å				
			c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_08				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)				
			c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_09				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å				
			c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)				
Occupancy Parameter			oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_10
Space Group	I – 4
Scale	0.0000001(3)
Lattice Parameter	a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å
	c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å

Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.00000912(6)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.250

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name			LiNH2_00				
Space Group			I – 4				
Scale			0.0000010(2)				
Lattice Parameter			a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å				
			c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å				
Occupancy Parameter			oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)				
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)

Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ	0.982(9)	b_{eq}= 0.1(3)

					(oLi07)		
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_06
Space Group	I – 4
Scale	0.0000010(3)
Lattice Parameter	a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å
	c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å
Occupancy	oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)

Parameter							
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_09
Space Group	I – 4
Scale	0.0000010(3)

Lattice Parameter			a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å				
			c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å				
Occupancy Parameter			oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)				
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name			LiNH2_10				
Space Group			I – 4				
Scale			0.0000010(2)				
Lattice Parameter			a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å				
			c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å				
Occupancy Parameter			oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)				
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000119(2)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.0000548(2)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810

Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å				
			c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_02
Space Group	I – 4
Scale	0.0000001(3)

Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_03				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å				
			c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_04				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å				
			c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_05
Space Group	I – 4
Scale	0.0000001(3)
Lattice Parameter	a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å
	c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å

Nitrogen Z Coordinate			z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_06				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å				
			c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_07				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å				
			c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_08
Space Group	I – 4
Scale	0.0000001(3)
Lattice Parameter	a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)
	c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å
Nitrogen Z Coordinate	z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)
Occupancy Parameter	oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)

Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_09				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å				
			c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)				
Occupancy Parameter			oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_10				
Space Group			I – 4				
Scale			0.0000002(3)				
Lattice Parameter			a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å				
			c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.00002015(8)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.167

R_ expected	8.132	R_expected'	17.074
R_weighted pattern	17.815	R_weighted pattern'	37.408
R_Pattern	13.547	R_Pattern'	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name		LiNH2_00					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)

Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_0 + 0.2*aLi_{10} = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-	0.02(1)	b_{eq}= 0.1(3)

					oLi04)		
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)

Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_10
Space Group	I – 4
Scale	0.0000010(2)
Lattice Parameter	a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å
	c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å

Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000029(1)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.00000072(5)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name	Li3Na(NH2)4_00
Space Group	I – 4
Scale	0.0000001(2)
Lattice Parameter	a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å

			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å				
			c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_02				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å				
			c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)				
Occupancy Parameter			oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_03
Space Group	I – 4
Scale	0.0000001(2)
Lattice Parameter	a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å
	c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å
Nitrogen Z Coordinate	z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)

Occupancy Parameter			oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_04				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å				
			c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)				
Occupancy Parameter			oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_05				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å				
			c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_06				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å				
			c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484

Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_07					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å					
		c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)					
Occupancy Parameter		oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_08					
Space Group		I – 4					
Scale		0.0000001(2)					
Lattice Parameter		a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)					
		c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)					
Occupancy Parameter		oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_09					
Space Group		I – 4					
Scale		0.0000001(2)					
Lattice Parameter		a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å					
		c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)					
Occupancy Parameter		oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484

Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_10				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å				
			c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.00000072(5)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0.083

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name	LiNH2_00
Space Group	I – 4

Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å					
		c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å					
Occupancy Parameter		oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_01					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å					
		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_04					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)

Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)

Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_10					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name			Li2O				
Space Group			Fm3m				
Scale			0.000105(2)				
Lattice Parameter			a = b = c = 4.6113(1) Å				
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name			LiNa2(NH2)3				
Space Group			P42/m				
Scale			0.00000010(6)				
Lattice Parameter			a = b = 6.28325(1)Å				
			c = 11.14942(2)Å				
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_0 = 0.1012(2)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	z_N_{10} = 0.1012(8)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_0 = 0.960(6)
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	yNa_{10} = 0.748(2)

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			a = b = a_ 00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)Å				
			c = c_ 00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 1.0* z_N_0 + 0.0* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa00= 1.0* yNa_0 + 0.0*yNa_{10} = 0.960(6)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)Å				
			c = c_ 01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2) Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.9* z_N_0 + 0.1* z_N_{10} = 0.1012(3)				
Occupancy Parameter			oNa01= 0.9* yNa_0 + 0.1*yNa_{10} = 0.939(7)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484

Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_02					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)Å					
		c = c_ 02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.8* z_N_0 + 0.2* z_N_{10} =0.1012(3)					
Occupancy Parameter		oNa02= 0.8* yNa_0 + 0.2*yNa_{10} = 0.918(9)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_03					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å					
		c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)					
Occupancy Parameter		oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_04					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å					
		c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)					
Occupancy Parameter		oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484

Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_05					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		$a = b = a_05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)$Å					
		$c = c_05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.5*\ z\_N_0 + 0.5*\ z\_N_{10} = 0.1012(5)$					
Occupancy Parameter		$oNa05 = 0.5*\ yNa_0 + 0.5*yNa_{10} = 0.85(1)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_06					
Space Group		I – 4					
Scale		0.0000001(4)					
Lattice Parameter		$a = b = a_06 = 0.4*a_{10} + 0.6*a_{10} = 5.0729(3)$Å					
		$c = c_06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.4*\ z\_N_0 + 0.6*\ z\_N_{10} = 0.1012(5)$					
Occupancy Parameter		$oNa06 = 0.4*\ yNa_0 + 0.6*yNa_{10} = 0.83(1)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_07					
Space Group		I – 4					
Scale		0.0000001(4)					
Lattice Parameter		$a = b = a_07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)$Å					
		$c = c_07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.3*\ z\_N_0 + 0.7*\ z\_N_{10} = 0.1012(6)$					
Occupancy Parameter		$oNa07 = 0.3*\ yNa_0 + 0.7*yNa_{10} = 0.81(1)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484

Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_08					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		$a = b = a\_08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)$					
		$c = c_08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.2*\ z\_N_0 + 0.8*\ z\_N_{10} = 0.1012(6)$					
Occupancy Parameter		$oNa08= 0.2*\ yNa_0 + 0.8*yNa_{10} = 0.79(2)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_09					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		$a = b = a_09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)$Å					
		$c = c_09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.1*\ z\_N_0 + 0.9*\ z\_N_{10} = 0.1012(7)$					
Occupancy Parameter		$oNa09= 0.1*\ yNa_0 + 0.9*yNa_{10} = 0.77(2)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_10					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		$a = b = a_10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)$Å					
		$c = c_10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)$Å					
Nitrogen Z Coordinate		$z\_N = z\_N_0 = 0.0*\ z\_N_0 + 1.0*\ z\_N_{10} = 0.1012(8)$					
Occupancy Parameter		$oNa10= 0.0*\ yNa_0 + 1.0*yNa_{10} = 0.75(2)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.0000408(1)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556

x = 0

R_ expected	8.132	R_expected’	17.074
R_weighted pattern	17.815	R_weighted pattern’	37.408
R_Pattern	13.547	R_Pattern’	42.758
Weighted_Durbin_Watson	12.699		
Goodness of fit	2.191		

LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_0 = 5.03648(2)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	aLi_{10} = 5.04770(7)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_0 = 10.25325(6)Å
LiNH2_00 – LiNH2_10 Lattice Parameter	cLi_{10} = 10.3547(2)Å
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_0 = 0.982(7)
LiNH2_00 – LiNH2_10 Occ. Parameter	wLi_{10} = 0.98(1)

Phase Name			LiNH2_00				
Space Group			I – 4				
Scale			0.0000010(3)				
Lattice Parameter			a = b = a_liam_00 = 1.0*aLi_0 + 0.0*aLi_{10} = 5.03648(2)Å				
			c = c_liam_00 = 1.0*cLi_0 + 0.0*cLi_{10} = 10.25325(6)Å				
Occupancy Parameter			oLi00 = 1.0* yLi_0 + 0.0*yLi_{10} = 0.982(7)				
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi00)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi00)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2327(3)	-0.2398(7)	-0.1146(1)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_01
Space Group	I – 4
Scale	0.0000010(3)
Lattice Parameter	a = b = a_liam_01 = 0.9*aLi_0 + 0.1*aLi_{10} = 5.03760(3)Å

		c = c_liam_01 = 0.9*cLi_0 + 0.1*cLi_{10} = 10.26340(8)Å					
Occupancy Parameter		oLi01= 0.9* yLi_0 + 0.1*yLi_{10} = 0.982(7)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi01)	0.982(7)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi01)	0.018(7)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_02					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_02 = 0.8*aLi_{10} + 0.2*aLi_0 = 5.03872(3)Å					
		c = c_liam_02 = 0.8*cLi_0 + 0.2*cLi_{10} = 10.27354(9)Å					
Occupancy Parameter		oLi02= 0.8* yLi_0 + 0.2*yLi_{10} = 0.982(8)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi02)	0.982(8)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi02)	0.018(8)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_03					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_03 = 0.7*aLi_0 + 0.3*aLi_{10} = 5.03985(4) Å					
		c = c_liam_03 = 0.7*cLi_0 + 0.3*cLi_{10} = 10.2837(1)Å					
Occupancy Parameter		oLi03= 0.7* yLi_0 + 0.3*yLi_{10} = 0.982(9)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.982(9)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.018(9)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name	LiNH2_04

Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_04 = 0.6*aLi_0 + 0.4*aLi_{10} = 5.04097(4)Å					
		c = c_liam_04 = 0.6*cLi_0 + 0.4*cLi_{10} = 10.2938(1)Å					
Occupancy Parameter		oLi04= 0.6* yLi_0 + 0.4*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi04)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi04)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_05					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_05 = 0.5*aLi_0 + 0.5*aLi_{10} = 5.04209(5)Å					
		c = c_liam_05 = 0.5*cLi_0 + 0.5*cLi_{10} = 10.3040(1)Å					
Occupancy Parameter		oLi05= 0.5* yLi_0 + 0.5*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi05)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi05)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_06					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_06 = 0.4*aLi_0 + 0.6*aLi_{10} = 5.04321(5)Å					
		c = c_liam_06 = 0.4*cLi_0 + 0.6*cLi_{10} = 10.3141(2)Å					
Occupancy Parameter		oLi06= 0.4* yLi_0 + 0.6*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi06)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi06)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)

Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_07					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_07 = 0.3*aLi_0 + 0.7*aLi_{10} = 5.04433(6)Å					
		c = c_liam_07 = 0.3*cLi_0 + 0.7*cLi_{10} = 10.3243(2)Å					
Occupancy Parameter		oLi07= 0.3* yLi_0 + 0.7*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi07)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi07)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_08					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_08 = 0.2*aLi_0 + 0.8*aLi_{10} =5.04546(6) Å					
		c = c_liam_08 = 0.2*cLi_0 + 0.8*cLi_{10} = 10.3344(2)Å					
Occupancy Parameter		oLi08= 0.2* yLi_0 + 0.8*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi08)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi08)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_09					
Space Group		I – 4					
Scale		0.0000010(3)					
Lattice Parameter		a = b = a_liam_09 = 0.1*aLi_0 + 0.9*aLi_{10} = 5.04658(7)Å					
		c = c_liam_09 = 0.1*cLi_0 + 0.9*cLi_{10} = 10.3446(2)Å					
Occupancy Parameter		oLi09= 0.1* yLi_0 + 0.9*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi09)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi09)	0.02(1)	b_{eq}= 0.1(3)

Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		LiNH2_10					
Space Group		I – 4					
Scale		0.0000010(2)					
Lattice Parameter		a = b = a_liam_10 = 0.0*aLi_0 + 1.0*aLi_{10} = 5.04770(7)Å					
		c = c_liam_10 = 0.0*cLi_0 + 1.0*cLi_{10} = 10.3547(2)Å					
Occupancy Parameter		oLi10= 0.0* yLi_0 + 1.0*yLi_{10} = 0.98(1)					
Site	Li 1	0.0	0.0	0.0	occ	1	b_{eq}= 0.30(4)
Site	Li 2	0.0	0.5	-0.25	occ (oLi10)	0.98(1)	b_{eq}= 0.1(3)
Site	Na 2	0.0	0.5	-0.25	occ (1-oLi10)	0.02(1)	b_{eq}= 0.1(3)
Site	Li 3	0.0	0.5	0.00620	occ	1	b_{eq}= 0.30(4)
Site	N	-0.2303(1)	-0.2407(3)	-0.11436(4)	occ	1	b_{eq}= 0.30(4)
Site	H 1	-0.226	-0.149	-0.172	occ	1	b_{eq}= 0.30(4)
Site	H 2	-0.308	-0.359	-0.114	occ	1	b_{eq}= 0.30(4)

Phase Name		Li2O					
Space Group		Fm3m					
Scale		0.000004(2)					
Lattice Parameter		a = b = c = 4.6113(1) Å					
Site	Li	0.25	0.25	0.25	occ	1	b_{eq} = 0.9148
Site	O	0.0	0.0	0.0	occ	1	b_{eq} = 0.8

Phase Name		LiNa2(NH2)3					
Space Group		P42/m					
Scale		0.0000001(6)					
Lattice Parameter		a = b = 6.28325(1)Å					
		c = 11.14942(2)Å					
Site	N 1	0.66317	0.27595	0.0	occ	1	b_{eq} = 1.5810
Site	H 1	0.73697	0.29827	0.056	occ	1	b_{eq} = 1.5810
Site	N 2	0.20732	0.27336	0.15765	occ	1	b_{eq} = 1.5810
Site	H 2	0.16362	0.18116	0.21186	occ	1	b_{eq} = 1.5810
Site	H 3	0.10362	0.32316	0.14126	occ	1	b_{eq} = 1.5810
Site	Na 1	0.50	0.0	0.14216	occ	1	b_{eq} = 2.2740
Site	Na 2	0.0	0.0	0.0	occ	1	b_{eq} = 2.2740
Site	Na 3	0.50	0.50	0.25	occ	1	b_{eq} = 2.2740
Site	Li 1	0.35356	0.36094	0.0	occ	1	b_{eq} = 2.0455

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_0 = 5.0830(4)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	a_{10} = 5.0662(2)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_0 = 11.5349(1)Å
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	c_{10} = 11.2957(7)Å

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	$z\_N_0 = 0.1012(2)$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	$z\_N_{10} = 0.1012(8)$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	$yNa_0 = 0.960(6)$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	$yNa_{10} = 0.748(2)$

Phase Name			Li3Na(NH2)4_00				
Space Group			I – 4				
Scale			0.0000001(2)				
Lattice Parameter			$a = b = a_00 = 1.0*a_0 + 0.0*a_{10} = 5.0830(4)$Å				
			$c = c_00 = 1.0*c_0 + 0.0*c_{10} = 11.5349(1)$Å				
Nitrogen Z Coordinate			$z\_N = z\_N_0 = 1.0*\ z\_N_0 + 0.0*\ z\_N_{10} = 0.1012(3)$				
Occupancy Parameter			$oNa00 = 1.0*\ yNa_0 + 0.0*yNa_{10} = 0.960(6)$				
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.960(6)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.040(6)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	Occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	Occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	Occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_01				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			$a = b = a_01 = 0.9*a_0 + 0.1*a_{10} = 5.0813(4)$Å				
			$c = c\_01 = 0.9*c_0 + 0.1*c_{10} = 11.5110(2)$ Å				
Nitrogen Z Coordinate			$z\_N = z\_N_0 = 0.9*\ z\_N_0 + 0.1*\ z\_N_{10} = 0.1012(3)$				
Occupancy Parameter			$oNa01 = 0.9*\ yNa_0 + 0.1*yNa_{10} = 0.939(7)$				
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.939(7)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.061(7)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_02				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			$a = b = a_02 = 0.8*a_{10} + 0.2*a_{10} = 5.0796(4)$Å				
			$c = c_02 = 0.8*c_{10} + 0.2*c_{10} = 11.4871(3)$Å				
Nitrogen Z Coordinate			$z\_N = z\_N_0 = 0.8*\ z\_N_0 + 0.2*\ z\_N_{10} = 0.1012(3)$				
Occupancy Parameter			$oNa02 = 0.8*\ yNa_0 + 0.2*yNa_{10} = 0.918(9)$				
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.918(9)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.092(9)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(3)	occ	1	b_{eq} 2.2484

Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_03					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 03 = 0.7*a_{10} + 0.3*a_{10} = 5.0780(3)Å					
		c = c_ 03 = 0.7*c_{10} + 0.3*c_{10} = 11.4632(3)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.7* z_N_0 + 0.3* z_N_{10} = 0.1012(4)					
Occupancy Parameter		oNa03= 0.7* yNa_0 + 0.3*yNa_{10} = 0.90(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.90(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.10(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_04					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 04 = 0.6*a_{10} + 0.4*a_{10} =5.0746(3) Å					
		c = c_ 04 = 0.6*c_{10} + 0.4*c_{10} = 11.4392(4)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.6* z_N_0 + 0.4* z_N_{10} = 0.1012(4)					
Occupancy Parameter		oNa04= 0.6* yNa_0 + 0.4*yNa_{10} = 0.88(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.88(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.12(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(4)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name		Li3Na(NH2)4_05					
Space Group		I – 4					
Scale		0.0000001(3)					
Lattice Parameter		a = b = a_ 05 = 0.5*a_{10} + 0.5*a_{10} = 5.0746(3)Å					
		c = c_ 05 = 0.5*c_{10} + 0.5*c_{10} = 11.4153(4)Å					
Nitrogen Z Coordinate		z_N = z_N_0 = 0.5* z_N_0 + 0.5* z_N_{10} = 0.1012(5)					
Occupancy Parameter		oNa05= 0.5* yNa_0 + 0.5*yNa_{10} = 0.85(1)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_05)	0.85(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_05)	0.15(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_06				
Space Group			I – 4				
Scale			0.0000001(4)				
Lattice Parameter			a = b = a_ 06 = 0.4*a_{10} + 0.6*a_{10} =5.0729(3)Å				
			c = c_ 06 = 0.4*c_{10} + 0.6*c_{10} = 11.3914(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.4* z_N_0 + 0.6* z_N_{10} = 0.1012(5)				
Occupancy Parameter			oNa06= 0.4* yNa_0 + 0.6*yNa_{10} = 0.83(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_06)	0.83(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_06)	0.17(3)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(5)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_07				
Space Group			I – 4				
Scale			0.0000001(4)				
Lattice Parameter			a = b = a_ 07 = 0.3*a_{10} + 0.7*a_{10} = 5.0713(3)Å				
			c = c_ 07 = 0.3*c_{10} + 0.7*c_{10} = 11.3675(5)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.3* z_N_0 + 0.7* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa07= 0.3* yNa_0 + 0.7*yNa_{10} = 0.81(1)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_07)	0.81(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_07)	0.19(1)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_08				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 08 = 0.2*a_{10} + 0.8*a_{10} = 5.0696(2)				
			c = c_ 08 = 0.2*c_{10} + 0.8*c_{10} = 11.3436(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.2* z_N_0 + 0.8* z_N_{10} = 0.1012(6)				
Occupancy Parameter			oNa08= 0.2* yNa_0 + 0.8*yNa_{10} = 0.79(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.79(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.21(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(6)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name	Li3Na(NH2)4_09

Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 09 = 0.1*a_{10} + 0.9*a_{10} = 5.0679(2)Å				
			c = c_ 09 = 0.1*c_{10} + 0.9*c_{10} = 11.3196(6)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.1* z_N_0 + 0.9* z_N_{10} = 0.1012(7)				
Occupancy Parameter			oNa09= 0.1* yNa_0 + 0.9*yNa_{10} = 0.77(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.77(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.23(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(7)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			Li3Na(NH2)4_10				
Space Group			I – 4				
Scale			0.0000001(3)				
Lattice Parameter			a = b = a_ 10 = 0.0*a_{10} + 1.0*a_{10} = 5.0662(2)Å				
			c = c_ 10 = 0.0*c_{10} + 1.0*c_{10} = 11.2957(7)Å				
Nitrogen Z Coordinate			z_N = z_N_0 = 0.0* z_N_0 + 1.0* z_N_{10} = 0.1012(8)				
Occupancy Parameter			oNa10= 0.0* yNa_0 + 1.0*yNa_{10} = 0.75(2)				
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.75(2)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.25(2)	b_{eq} 2.2484
Site	Li 2	0.0	0.0	0.0	occ	1	b_{eq} 2.2484
Site	Li 3	0.0	0.50	0.0087	occ	1	b_{eq} 2.2484
Site	N	0.250(1)	0.248(2)	0.1012(8)	occ	1	b_{eq} 2.2484
Site	H 1	0.365	0.290	0.110	occ	1	b_{eq} 2.2484
Site	H 2	0.233	0.139(6)	0.168(3)	occ	1	b_{eq} 2.2484

Phase Name			NaNH2				
Space Group			Fddd				
Scale			0.0000422(1)				
Lattice Parameter			a = 8.95918(2) Å				
			b = 10.45229(3) Å				
			c = 8.07224(2) Å				
Site	Na 1	0.0	0.14841	0.0	occ	1	b_{eq} 2.6283
Site	N	0.0	0.0	0.23425	occ	1	b_{eq} 3.2183
Site	H 1	0.05938	0.95625	0.29968	occ	1	b_{eq} 2.7556