

The Synthesis and Structural Investigation of Mixed Lithium / Sodium Amides

Rebecca L. Lowton, Martin O. Jones, William I. F. David, Simon R. Johnson, Marco Sommariva, and
Peter. P. Edwards

Supplementary Crystallographic Information for System III

$$x = 0.75$$

R _{expected}	5.199	R _{expected} '	10.258
R _{weighted pattern}	9.782	R _{weighted pattern} '	19.302
R _{Pattern}	8.662	R _{Pattern} '	26.702
Weighted _{Durbin} _{Watson}	1.109		
Goodness of fit	1.882		

Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	$a_0 = 5.08337(9)\text{\AA}$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	$a_{10} = 5.0717(6)\text{\AA}$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	$c_0 = 11.5265(3)\text{\AA}$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	$c_{10} = 11.375(2)\text{\AA}$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	$z_{N_0} = 0.991(3)$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Lattice Parameter	$z_{N_{10}} = 0.109(2)$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	$y_{Na_0} = 0.93(1)$
Li3Na(NH2)4_00 – Li3Na(NH2)4_10 Occ. Parameter	$y_{Na_{10}} = 0.93(6)$

Phase Name		Li3Na(NH2)4_00					
Space Group		I – 4					
Scale		0.000082(3)					
Lattice Parameter		$a = b = a_{00} = 1.0*a_0 + 0.0*a_{10} = 5.08334(9)\text{\AA}$					
		$c = c_{00} = 1.0*c_0 + 0.0*c_{10} = 11.5265(3)\text{\AA}$					
Nitrogen Z Coordinate		$z_N = z_{N_0} = 1.0*z_{N_0} + 0.0*z_{N_{10}} = 0.0992(3)$					
Occupancy Parameter		$o_{Na00} = 1.0*y_{Na_0} + 0.0*y_{Na_{10}} = 0.93(1)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_00)	0.93(1)	b_{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_00)	0.07(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	0.238(4)	0.2360(5)	0.0992(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		0.000409(5)					
Lattice Parameter		$a = b = a_{01} = 0.9*a_0 + 0.1*a_{10} = 5.0822(1)\text{\AA}$					
		$c = c_{01} = 0.9*c_0 + 0.1*c_{10} = 11.5114(4)\text{\AA}$					
Nitrogen Z Coordinate		$z_N = z_{N_0} = 0.9*z_{N_0} + 0.1*z_{N_{10}} = 0.1001(4)$					
Occupancy Parameter		$o_{Na01} = 0.9*y_{Na_0} + 0.1*y_{Na_{10}} = 0.93(2)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_01)	0.93(2)	b_{eq} 2.2484

Site	Li 1	0.0	0.50	0.25	occ (1-oNa_01)	0.07(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	0.238(4)	0.2360(5)	0.1001(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		Li ₃ Na(NH ₂) ₄ _02					
Space Group		I – 4					
Scale		0.000214(3)					
Lattice Parameter		a = b = a _{_02} = 0.8*a ₁₀ + 0.2*a ₁₀ = 5.0810(2) Å					
		c = c _{_02} = 0.8*c ₁₀ + 0.2*c ₁₀ = 11.4963(6) Å					
Nitrogen Z Coordinate		z _N = z _{N₀} = 0.8* z _{N₀} + 0.2* z _{N₁₀} = 0.1011(6)					
Occupancy Parameter		oNa02= 0.8* yNa ₀ + 0.2*yNa ₁₀ = 0.93(2)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_02)	0.93(2)	b _{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_02)	0.07(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	0.238(4)	0.2360(5)	0.1011(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		Li ₃ Na(NH ₂) ₄ _03					
Space Group		I – 4					
Scale		0.000035(2)					
Lattice Parameter		a = b = a _{_03} = 0.7*a ₁₀ + 0.3*a ₁₀ = 5.0799(2) Å					
		c = c _{_03} = 0.7*c ₁₀ + 0.3*c ₁₀ = 11.4811(7) Å					
Nitrogen Z Coordinate		z _N = z _{N₀} = 0.7* z _{N₀} + 0.3* z _{N₁₀} = 0.1021(7)					
Occupancy Parameter		oNa03= 0.7* yNa ₀ + 0.3*yNa ₁₀ = 0.93(3)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_03)	0.93(3)	b _{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_03)	0.07(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	0.238(4)	0.2360(5)	0.1121(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		Li ₃ Na(NH ₂) ₄ _04					
Space Group		I – 4					
Scale		0.000003(1)					
Lattice Parameter		a = b = a _{_04} = 0.6*a ₁₀ + 0.4*a ₁₀ = 5.0787(3) Å					
		c = c _{_04} = 0.6*c ₁₀ + 0.4*c ₁₀ = 11.4660(9) Å					
Nitrogen Z Coordinate		z _N = z _{N₀} = 0.6* z _{N₀} + 0.4* z _{N₁₀} = 0.1031(9)					
Occupancy Parameter		oNa04= 0.6* yNa ₀ + 0.4*yNa ₁₀ = 0.93(3)					
Site	Na 1	0.0	0.50	0.25	occ (oNa_04)	0.93(3)	b _{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_04)	0.07(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	0.238(4)	0.2360(5)	0.1031(9)	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		0.000000(1)					
Lattice Parameter		a = b = a ₀₅ = 0.5*a ₁₀ + 0.5*a ₁₀ = 5.0775(3)Å					
		c = c ₀₅ = 0.5*c ₁₀ + 0.5*c ₁₀ = 11.451(1)Å					
Nitrogen Z Coordinate		z _N = z _{N0} = 0.5* z _{N0} + 0.5* z _{N10} = 0.104(1)					
Occupancy Parameter		oNa05= 0.5* yNa ₀ + 0.5*yNa ₁₀ = 0.93(4)					
Site	Na 1	0.0	0.50	0.25	occ (oNa ₀₅)	0.93(4)	b _{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa ₀₅)	0.07(4)	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	0.238(4)	0.2360(5)	0.104(1)	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		0.000000(1)					
Lattice Parameter		a = b = a ₀₆ = 0.4*a ₁₀ + 0.6*a ₁₀ = 5.0764(4)Å					
		c = c ₀₆ = 0.4*c ₁₀ + 0.6*c ₁₀ = 11.436(1)Å					
Nitrogen Z Coordinate		z _N = z _{N0} = 0.4* z _{N0} + 0.6* z _{N10} = 0.105(1)					
Occupancy Parameter		oNa06= 0.4* yNa ₀ + 0.6*yNa ₁₀ = 0.94(4)					
Site	Na 1	0.0	0.50	0.25	occ (oNa ₀₆)	0.93(4)	b _{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa ₀₆)	0.07(4)	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	0.238(4)	0.2360(5)	0.105(1)	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(9)					
Lattice Parameter		a = b = a ₀₇ = 0.3*a ₁₀ + 0.7*a ₁₀ = 5.0752(4)Å					
		c = c ₀₇ = 0.3*c ₁₀ + 0.7*c ₁₀ = 11.421(1)Å					
Nitrogen Z Coordinate		z _N = z _{N0} = 0.3* z _{N0} + 0.7* z _{N10} = 0.106(1)					
Occupancy Parameter		oNa07= 0.3* yNa ₀ + 0.7*yNa ₁₀ = 0.93(5)					
Site	Na 1	0.0	0.50	0.25	occ (oNa ₀₇)	0.93(5)	b _{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa ₀₇)	0.07(5)	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	0.238(4)	0.2360(5)	0.106(1)	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(8)					
Lattice Parameter		$a = b = a_{08} = 0.2 \cdot a_{10} + 0.8 \cdot a_{10} = 5.741(5) \text{ \AA}$					
		$c = c_{08} = 0.2 \cdot c_{10} + 0.8 \cdot c_{10} = 11.405(1) \text{ \AA}$					
Nitrogen Z Coordinate		$z_N = z_{N_0} = 0.2 \cdot z_{N_0} + 0.8 \cdot z_{N_{10}} = 0.107(1)$					
Occupancy Parameter		$oNa_{08} = 0.2 \cdot y_{Na_0} + 0.8 \cdot y_{Na_{10}} = 0.93(6)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_08)	0.93(6)	b _{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_08)	0.07(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	0.238(4)	0.2360(5)	0.107(1)	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(7)					
Lattice Parameter		$a = b = a_{09} = 0.1 \cdot a_{10} + 0.9 \cdot a_{10} = 5.0729(5) \text{ \AA}$					
		$c = c_{09} = 0.1 \cdot c_{10} + 0.9 \cdot c_{10} = 11.390(3) \text{ \AA}$					
Nitrogen Z Coordinate		$z_N = z_{N_0} = 0.1 \cdot z_{N_0} + 0.9 \cdot z_{N_{10}} = 0.1079(2)$					
Occupancy Parameter		$oNa_{09} = 0.1 \cdot y_{Na_0} + 0.9 \cdot y_{Na_{10}} = 0.93(6)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_09)	0.93(6)	b _{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_09)	0.07(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	0.238(4)	0.2360(5)	0.108(2)	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(5)					
Lattice Parameter		$a = b = a_{10} = 0.0 \cdot a_{10} + 1.0 \cdot a_{10} = 5.0717(6) \text{ \AA}$					
		$c = c_{10} = 0.0 \cdot c_{10} + 1.0 \cdot c_{10} = 11.375(2) \text{ \AA}$					
Nitrogen Z Coordinate		$z_N = z_{N_0} = 0.0 \cdot z_{N_0} + 1.0 \cdot z_{N_{10}} = 0.109(2)$					
Occupancy Parameter		$oNa_{10} = 0.0 \cdot y_{Na_0} + 1.0 \cdot y_{Na_{10}} = 0.93(7)$					
Site	Na 1	0.0	0.50	0.25	occ (oNa_10)	0.93(7)	b _{eq} 2.2484
Site	Li 1	0.0	0.50	0.25	occ (1-oNa_10)	0.07(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	0.238(4)	0.2360(5)	0.109(2)	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		Li ₂ O					
Space Group		Fm3m					
Scale		0.000167(4)					
Lattice Parameter		a = b = c = 4.6218(3) 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		LiNa ₂ (NH ₂) ₃					
Space Group		P4 ₂ /m					
Scale		0.0000187(2)					
Lattice Parameter		a = b = 6.28484(9) Å					
		c = 11.15341(3) 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

x = 0.333

R _{expected}	4.158	R _{expected} '	7.024
R _{weighted pattern}	10.40	R _{weighted pattern} '	17.567
R _{Pattern}	8.747	R _{Pattern} '	21.500
Weighted_Durbin_Watson	0.918		
Goodness of fit	2.051		

Phase Name		Li ₂ O					
Space Group		Fm3m					
Scale		0.000470(6)					
Lattice Parameter		a = b = c = 4.6176(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		LiNa ₂ (NH ₂) ₃					
Space Group		P4 ₂ /m					
Scale		0.00034(1)					
Lattice Parameter		a = b = 6.28309(1) Å					
		c = 11.14687(3) 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	$b_{eq} = 2.0455$

Phase Name		NaNH ₂					
Space Group		Fddd					
Scale		0.0000222(2)					
Lattice Parameter		a = 8.9593(2) Å					
		b = 10.4487(2) Å					
		c = 8.0732(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	$b_{eq} 2.7556$