Supplement A

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2 x\ 10^3$) for Pandian 1746. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

x	y	z	U(eq)	
C(1)	10573(3)	9600(3)	168(2)	83(1)
C(2)	10756(3)	8751(3)	377(2)	84(1)
C(3)	11641(3)	8779(3)	505(2)	86(1)
C(4)	11946(3)	9638(3)	362(2)	83(1)
C(5)	13066(3)	10677(3)	297(2)	86(1)
C(6)	13983(3)	10921(4)	308(2)	96(2)
C(7)	14015(3)	11809(4)	215(2)	96(2)
C(8)	13102(3)	12066(4)	120(2)	92(1)
C(9)	10241(4)	8032(3)	464(2)	90(1)
C(10)	10646(4)	7275(3)	659(2)	94(1)
C(11)	10160(4)	6516(4)	747(2)	106(2)
C(12)	10534(5)	5797(4)	932(2)	116(2)
C(13)	11379(5)	5820(4)	1054(2)	120(2)
C(14)	11910(5)	6537(4)	984(2)	116(2)
C(15)	11520(4)	7301(3)	784(2)	96(1)
C(16)	12023(4)	8069(3)	708(2)	93(1)
C(17)	14740(4)	10449(4)	407(2)	98(2)
C(18)	15526(4)	10908(5)	427(2)	105(2)
C(19)	16308(4)	10477(5)	524(2)	119(2)
C(20)	17062(5)	10926(7)	549(2)	139(3)
C(21)	17102(4)	11803(7)	450(2)	139(3)
C(22)	16358(4)	12265(5)	351(2)	124(2)
C(23)	15550(3)	11804(5)	333(2)	107(2)
C(24)	14777(4)	12264(4)	224(2)	109(2)
Li	11315(5)	11315(5)	0	84(3)
N(1)	11292(3)	10101(2)	171(1)	83(1)
N(2)	12770(3)	9892(3)	416(1)	91(1)
N(3)	12569(3)	11377(3)	179(1)	89(1)
N(4)	12868(3)	12868(3)	0	96(2)
N(5)	9791(3)	9791(3)	0	83(1)

O(1)	9380(2)	7984(2)	365(1)	93(1)
O(2)	12880(2)	8072(2)	845(1)	100(1)
O(3)	14775(2)	9603(3)	496(1)	115(1)
O(4)	14837(3)	13135(3)	139(2)	127(1)
C(25)	8840(4)	8451(4)	685(2)	112(2)
C(26)	7903(6)	8169(6)	645(3)	157(3)
C(27)	7755(6)	7228(6)	706(3)	161(3)
C(28)	6803(8)	7022(12)	643(6)	297(8)
C(29)	12969(4)	8402(4)	1316(2)	105(2)
C(30)	13901(4)	8450(3)	1441(2)	105(2)
C(31)	14346(4)	7582(4)	1467(2)	106(2)
C(32)	15295(4)	7653(5)	1634(2)	126(2)
C(33)	14448(4)	9019(4)	146(3)	128(2)
C(34)	15008(5)	8288(6)	109(3)	159(3)
C(35)	14652(6)	7554(6)	-201(4)	181(4)
C(36)	14586(8)	7834(7)	-691(5)	235(6)
C(37)	14730(8)	13327(7)	-376(3)	123(4)*
C(38)	15182(9)	14161(7)	-544(4)	146(5)*
C(40)	15420(8)	15244(9)	-1155(4)	138(5)*
C(37A)	14447(9)	13625(8)	542(4)	118(5)*
C(38A)	14437(9)	14980(9)	-675(4)	127(5)*
C(40A)	15460(20)	13711(15)	-896(10)	283(16)*
C(39)	14996(5)	14491(7)	-1036(3)	165(3)

*Two orientations of a disordered n-butyl group with occupancy factors of 0.544(9) for atoms C(37), C(38) and C(40), and 0.456(9) for atoms C(37A), C(38A) and C(40A). Atom C(40A) was refined isotropically. Atom C(39) is common to both orientations.

Table 2. Bond lengths [Å] and angles [°]

C(1)-N(5)	1.333(6)
C(1)-N(1)	1.353(6)
C(1)-C(2)	1.471(7)
C(2)-C(9)	1.389(7)
C(2)-C(3)	1.415(7)
C(3)-C(16)	1.375(7)
C(3)-C(4)	1.466(7)
C(4)-N(2)	1.340(6)
C(4)-N(1)	1.353(6)
C(5)-N(2)	1.339(6)
C(5)-N(3)	1.368(6)
C(5)-C(6)	1.465(7)
C(6)-C(7)	1.397(7)
C(6)-C(17)	1.407(8)
C(7)-C(24)	1.370(8)
C(7)-C(8)	1.489(7)
C(8)-N(4)	1.335(6)
C(8)-N(3)	1.355(7)
C(9)-O(1)	1.361(6)
C(9)-C(10)	1.438(7)
C(10)-C(15)	1.397(8)
C(10)-C(11)	1.414(8)
C(11)-C(12)	1.361(8)
C(11)-H(11)	0.9500
C(12)-C(13)	1.351(9)
C(12)-H(12)	0.9500
C(13)-C(14)	1.392(9)
C(13)-H(13)	0.9500
C(14)-C(15)	1.444(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.434(7)
C(16)-O(2)	1.381(6)
C(17)-O(3)	1.331(7)
C(17)-C(18)	1.406(8)

C(18)-C(19)	1.406(8)
C(18)-C(23)	1.411(9)
C(19)-C(20)	1.357(10)
C(19)-H(19)	0.9500
C(20)-C(21)	1.385(11)
C(20)-H(20)	0.9500
C(21)-C(22)	1.382(10)
C(21)-H(21)	0.9500
C(22)-C(23)	1.438(8)
C(22)-H(22)	0.9500
C(23)-C(24)	1.424(9)
C(24)-O(4)	1.369(7)
Li-N(1)	1.938(9)
Li-N(1)#1	1.938(9)
Li-N(3)	2.007(9)
Li-N(3)#1	2.007(9)
N(4)-C(8)#1	1.335(6)
N(5)-C(1)#1	1.333(6)
O(1)-C(25)	1.436(6)
O(2)-C(29)	1.455(6)
O(3)-C(33)	1.444(7)
O(4)-C(37A)	1.512(7)
O(4)-C(37)	1.522(7)
C(25)-C(26)	1.514(10)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.482(11)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.514(15)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.486(8)

C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-C(31)	1.508(7)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-C(32)	1.547(8)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.426(9)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.545(11)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.480(15)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.543(9)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-C(39)	1.533(9)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(40)-C(39)	1.378(14)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(37A)-C(38A)#1	1.548(19)
C(37A)-H(37C)	0.9900
C(37A)-H(37D)	0.9900

C(38A)-C(37A)#1	1.548(19)
C(38A)-C(39)	1.549(9)
C(38A)-H(38C)	0.9900
C(38A)-H(38D)	0.9900
C(40A)-C(39)	1.461(10)
C(40A)-H(40D)	0.9800
C(40A)-H(40E)	0.9800
C(40A)-H(40F)	0.9800
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(39)-H(39C)	0.9900
C(39)-H(39D)	0.9900

N(5)-C(1)-N(1)	128.3(4)
N(5)-C(1)-C(2)	121.3(4)
N(1)-C(1)-C(2)	110.4(4)
C(9)-C(2)-C(3)	122.0(4)
C(9)-C(2)-C(1)	132.6(5)
C(3)-C(2)-C(1)	105.4(4)
C(16)-C(3)-C(2)	120.0(5)
C(16)-C(3)-C(4)	134.6(5)
C(2)-C(3)-C(4)	105.4(4)
N(2)-C(4)-N(1)	126.9(4)
N(2)-C(4)-C(3)	122.5(4)
N(1)-C(4)-C(3)	110.6(4)
N(2)-C(5)-N(3)	126.0(4)
N(2)-C(5)-C(6)	123.8(4)
N(3)-C(5)-C(6)	110.0(5)
C(7)-C(6)-C(17)	121.2(5)
C(7)-C(6)-C(5)	106.5(4)
C(17)-C(6)-C(5)	132.3(6)
C(24)-C(7)-C(6)	122.0(5)
C(24)-C(7)-C(8)	132.7(6)
C(6)-C(7)-C(8)	105.2(5)
N(4)-C(8)-N(3)	126.5(5)
N(4)-C(8)-C(7)	123.4(5)

N(3)-C(8)-C(7)	110.0(5)
O(1)-C(9)-C(2)	124.3(4)
O(1)-C(9)-C(10)	117.6(5)
C(2)-C(9)-C(10)	118.1(5)
C(15)-C(10)-C(11)	119.3(5)
C(15)-C(10)-C(9)	119.9(5)
C(11)-C(10)-C(9)	120.8(5)
C(12)-C(11)-C(10)	121.4(6)
C(12)-C(11)-H(11)	119.3
C(10)-C(11)-H(11)	119.3
C(13)-C(12)-C(11)	119.4(6)
C(13)-C(12)-H(12)	120.3
C(11)-C(12)-H(12)	120.3
C(12)-C(13)-C(14)	123.5(5)
C(12)-C(13)-H(13)	118.2
C(14)-C(13)-H(13)	118.2
C(13)-C(14)-C(15)	117.5(6)
C(13)-C(14)-H(14)	121.3
C(15)-C(14)-H(14)	121.3
C(10)-C(15)-C(16)	120.4(5)
C(10)-C(15)-C(14)	118.9(6)
C(16)-C(15)-C(14)	120.7(6)
C(3)-C(16)-O(2)	122.0(5)
C(3)-C(16)-C(15)	119.5(5)
O(2)-C(16)-C(15)	118.5(4)
O(3)-C(17)-C(18)	116.8(5)
O(3)-C(17)-C(6)	125.5(5)
C(18)-C(17)-C(6)	117.6(6)
C(19)-C(18)-C(17)	120.7(7)
C(19)-C(18)-C(23)	118.7(6)
C(17)-C(18)-C(23)	120.6(6)
C(20)-C(19)-C(18)	120.4(7)
C(20)-C(19)-H(19)	119.8
C(18)-C(19)-H(19)	119.8
C(19)-C(20)-C(21)	121.7(7)
C(19)-C(20)-H(20)	119.1

C(21)-C(20)-H(20)	119.1
C(22)-C(21)-C(20)	120.7(7)
C(22)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(21)-C(22)-C(23)	118.2(7)
C(21)-C(22)-H(22)	120.9
C(23)-C(22)-H(22)	120.9
C(18)-C(23)-C(24)	120.7(5)
C(18)-C(23)-C(22)	120.1(6)
C(24)-C(23)-C(22)	119.2(7)
O(4)-C(24)-C(7)	123.9(6)
O(4)-C(24)-C(23)	118.2(5)
C(7)-C(24)-C(23)	117.8(6)
N(1)-Li-N(1)#1	91.8(5)
N(1)-Li-N(3)	89.89(16)
N(1)#1-Li-N(3)	178.2(5)
N(1)-Li-N(3)#1	178.2(5)
N(1)#1-Li-N(3)#1	89.89(16)
N(3)-Li-N(3)#1	88.5(5)
C(1)-N(1)-C(4)	108.3(4)
C(1)-N(1)-Li	124.4(4)
C(4)-N(1)-Li	126.9(4)
C(5)-N(2)-C(4)	124.0(4)
C(8)-N(3)-C(5)	108.1(4)
C(8)-N(3)-Li	126.3(4)
C(5)-N(3)-Li	124.5(4)
C(8)#1-N(4)-C(8)	124.7(6)
C(1)-N(5)-C(1)#1	122.1(6)
C(9)-O(1)-C(25)	113.9(4)
C(16)-O(2)-C(29)	111.0(4)
C(17)-O(3)-C(33)	117.6(5)
C(24)-O(4)-C(37A)	109.0(7)
C(24)-O(4)-C(37)	111.1(6)
O(1)-C(25)-C(26)	111.2(5)
O(1)-C(25)-H(25A)	109.4
C(26)-C(25)-H(25A)	109.4

O(1)-C(25)-H(25B)	109.4
C(26)-C(25)-H(25B)	109.4
H(25A)-C(25)-H(25B)	108.0
C(27)-C(26)-C(25)	114.9(7)
C(27)-C(26)-H(26A)	108.5
C(25)-C(26)-H(26A)	108.5
C(27)-C(26)-H(26B)	108.5
C(25)-C(26)-H(26B)	108.5
H(26A)-C(26)-H(26B)	107.5
C(26)-C(27)-C(28)	110.0(10)
C(26)-C(27)-H(27A)	109.7
C(28)-C(27)-H(27A)	109.7
C(26)-C(27)-H(27B)	109.7
C(28)-C(27)-H(27B)	109.7
H(27A)-C(27)-H(27B)	108.2
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
O(2)-C(29)-C(30)	109.6(5)
O(2)-C(29)-H(29A)	109.7
C(30)-C(29)-H(29A)	109.7
O(2)-C(29)-H(29B)	109.7
C(30)-C(29)-H(29B)	109.7
H(29A)-C(29)-H(29B)	108.2
C(29)-C(30)-C(31)	114.1(5)
C(29)-C(30)-H(30A)	108.7
C(31)-C(30)-H(30A)	108.7
C(29)-C(30)-H(30B)	108.7
C(31)-C(30)-H(30B)	108.7
H(30A)-C(30)-H(30B)	107.6
C(30)-C(31)-C(32)	112.5(5)
C(30)-C(31)-H(31A)	109.1
C(32)-C(31)-H(31A)	109.1

C(30)-C(31)-H(31B)	109.1
C(32)-C(31)-H(31B)	109.1
H(31A)-C(31)-H(31B)	107.8
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-O(3)	109.5(5)
C(34)-C(33)-H(33A)	109.8
O(3)-C(33)-H(33A)	109.8
C(34)-C(33)-H(33B)	109.8
O(3)-C(33)-H(33B)	109.8
H(33A)-C(33)-H(33B)	108.2
C(33)-C(34)-C(35)	114.0(7)
C(33)-C(34)-H(34A)	108.7
C(35)-C(34)-H(34A)	108.7
C(33)-C(34)-H(34B)	108.7
C(35)-C(34)-H(34B)	108.7
H(34A)-C(34)-H(34B)	107.6
C(36)-C(35)-C(34)	111.3(9)
C(36)-C(35)-H(35A)	109.4
C(34)-C(35)-H(35A)	109.4
C(36)-C(35)-H(35B)	109.4
C(34)-C(35)-H(35B)	109.4
H(35A)-C(35)-H(35B)	108.0
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
O(4)-C(37)-C(38)	114.9(7)
O(4)-C(37)-H(37A)	108.5
C(38)-C(37)-H(37A)	108.5

O(4)-C(37)-H(37B)	108.5
C(38)-C(37)-H(37B)	108.5
H(37A)-C(37)-H(37B)	107.5
C(39)-C(38)-C(37)	118.9(8)
C(39)-C(38)-H(38A)	107.6
C(37)-C(38)-H(38A)	107.6
C(39)-C(38)-H(38B)	107.6
C(37)-C(38)-H(38B)	107.6
H(38A)-C(38)-H(38B)	107.0
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
O(4)-C(37A)-C(38A)#1	112.5(9)
O(4)-C(37A)-H(37C)	109.1
C(38A)#1-C(37A)-H(37C)	109.1
O(4)-C(37A)-H(37D)	109.1
C(38A)#1-C(37A)-H(37D)	109.1
H(37C)-C(37A)-H(37D)	107.8
C(37A)#1-C(38A)-C(39)	111.0(10)
C(37A)#1-C(38A)-H(38C)	109.4
C(39)-C(38A)-H(38C)	109.4
C(37A)#1-C(38A)-H(38D)	109.4
C(39)-C(38A)-H(38D)	109.4
H(38C)-C(38A)-H(38D)	108.0
C(39)-C(40A)-H(40D)	109.5
C(39)-C(40A)-H(40E)	109.5
H(40D)-C(40A)-H(40E)	109.5
C(39)-C(40A)-H(40F)	109.5
H(40D)-C(40A)-H(40F)	109.5
H(40E)-C(40A)-H(40F)	109.5
C(40)-C(39)-C(38)	114.9(8)
C(40A)-C(39)-C(38A)	119.4(10)
C(40)-C(39)-H(39A)	108.5

C(38)-C(39)-H(39A)	108.5
C(40)-C(39)-H(39B)	108.5
C(38)-C(39)-H(39B)	108.5
H(39A)-C(39)-H(39B)	107.5
C(40A)-C(39)-H(39C)	107.5
C(38A)-C(39)-H(39C)	107.5
C(40A)-C(39)-H(39D)	107.5
C(38A)-C(39)-H(39D)	107.5
H(39C)-C(39)-H(39D)	107.0

Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + \ldots . + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	95(4)	74(3)	79(3)	3(2)	-3(2)	4(3)
C(2)	86(3)	80(3)	87(3)	1(2)	-12(2)	7(3)
C(3)	97(3)	81(3)	79(3)	-7(2)	-10(2)	15(3)
C(4)	89(3)	79(3)	81(3)	-5(2)	-6(2)	4(3)
C(5)	86(3)	88(4)	84(3)	-5(3)	-13(2)	12(3)
C(6)	79(3)	111(4)	99(4)	-5(3)	-9(3)	5(3)
C(7)	87(4)	110(4)	91(3)	-12(3)	-1(3)	-6(3)
C(8)	82(3)	96(4)	97(3)	-7(3)	-1(2)	0(3)
C(9)	107(4)	86(3)	78(3)	2(2)	-9(3)	13(3)
C(10)	118(4)	86(3)	77(3)	8(2)	-7(3)	4(3)
C(11)	128(4)	90(4)	100(4)	7(3)	-16(3)	4(3)
C(12)	146(6)	94(4)	109(4)	11(3)	-29(4)	0(4)
C(13)	179(7)	79(4)	100(4)	10(3)	-32(4)	14(4)
C(14)	158(5)	91(4)	99(4)	-2(3)	-37(4)	30(4)
C(15)	119(4)	86(3)	81(3)	0(2)	-16(3)	12(3)
C(16)	99(4)	90(4)	88(3)	-5(3)	-22(3)	19(3)
C(17)	87(4)	120(5)	88(3)	-13(3)	-7(3)	6(3)
C(18)	97(4)	138(5)	79(3)	-2(3)	-5(3)	5(4)
C(19)	82(4)	175(6)	100(4)	-8(4)	-5(3)	10(4)
C(20)	88(5)	221(9)	108(5)	6(5)	-1(3)	3(5)
C(21)	85(5)	223(9)	107(4)	-1(5)	6(3)	-24(6)
C(22)	94(4)	172(6)	107(4)	5(4)	1(3)	-18(4)
C(23)	74(4)	163(6)	85(3)	-1(4)	-2(3)	-11(4)
C(24)	100(4)	123(5)	104(4)	-6(3)	1(3)	-19(4)
Li	77(4)	77(4)	97(7)	-2(4)	2(4)	6(5)
N(1)	80(2)	79(2)	89(2)	4(2)	-8(2)	6(2)
N(2)	83(3)	95(3)	96(3)	-7(2)	-15(2)	12(2)
N(3)	86(3)	94(3)	86(2)	-8(2)	-9(2)	1(2)
N(4)	93(3)	93(3)	102(4)	-3(2)	3(2)	-7(3)
N(5)	86(2)	86(2)	78(3)	10(2)	-10(2)	12(3)
O(1)	99(2)	89(2)	90(2)	1(2)	-2(2)	1(2)

O(2)	107(3)	98(2)	96(2)	-4(2)	-22(2)	25(2)
O(3)	97(3)	125(3)	123(3)	-24(2)	-27(2)	26(2)
O(4)	111(3)	128(4)	142(4)	-4(3)	-2(3)	-25(3)
C(25)	105(4)	108(4)	122(4)	-15(3)	1(3)	3(3)
C(26)	175(8)	156(7)	139(6)	-13(5)	42(5)	18(6)
C(27)	165(8)	150(7)	168(7)	15(5)	38(5)	-24(6)
C(28)	177(11)	430(20)	283(16)	-78(16)	85(11)	-23(13)
C(29)	118(4)	107(4)	91(3)	-16(3)	-20(3)	22(3)
C(30)	124(4)	92(4)	97(3)	-2(3)	-13(3)	10(3)
C(31)	128(4)	101(4)	89(3)	-3(3)	-22(3)	12(3)
C(32)	112(4)	156(6)	109(4)	-10(4)	-27(3)	6(4)
C(33)	98(4)	125(5)	160(6)	-25(4)	-31(4)	38(4)
C(34)	144(6)	173(7)	159(6)	-26(6)	-10(5)	29(6)
C(35)	171(8)	149(7)	221(10)	-51(7)	-37(7)	25(6)
C(36)	263(13)	201(10)	240(12)	-15(9)	-141(11)	46(9)
C(37)	109(8)	129(9)	130(10)	1(7)	-1(7)	-24(7)
C(38)	149(11)	154(12)	134(11)	-43(9)	25(9)	-45(9)
C(40)	121(9)	163(12)	130(10)	26(8)	-21(7)	-30(9)
C(37A)	119(10)	105(9)	129(10)	6(8)	-7(8)	-5(8)
C(38A)	149(12)	133(12)	98(9)	26(8)	5(9)	-12(10)
C(39)	143(6)	240(10)	114(5)	-1(6)	-3(5)	-73(7)

Table 4. Calculated hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3).

x	y	z	U(eq)	
H(11)	9559	6508	675	127
H(12)	10204	5283	975	140
H(13)	11623	5320	1194	143
H(14)	12506	6524	1065	139
H(19)	16308	9869	573	143
H(20)	17577	10630	637	167
H(21)	17647	12089	450	166
H(22)	16380	12872	296	149
H(25A)	8884	9080	620	134
H(25B)	9047	8349	1005	134
H(26A)	7560	8485	881	188
H(26B)	7683	8343	336	188
H(27A)	7944	7048	1020	193
H(27B)	8101	6901	476	193
H(28A)	6712	6397	676	445
H(28B)	6616	7207	334	445
H(28C)	6464	7330	879	445
H(29A)	12663	8014	1535	127
H(29B)	12705	8985	1337	127
H(30A)	13956	8741	1746	125
H(30B)	14204	8813	1209	125
H(31A)	14337	7309	1156	127
H(31B)	14021	7201	1681	127
H(32A)	15555	7074	1646	188
H(32B)	15307	7912	1945	188
H(32C)	15624	8019	1419	188
H(33A)	13857	8825	231	154
H(33B)	14415	9321	-156	154
H(34A)	15114	8053	424	190
H(34B)	15572	8482	-17	190
H(35A)	15040	7045	-180	217

H(35B)	14073	7379	-88	217
H(36A)	14348	7360	-878	352
H(36B)	15163	7987	-807	352
H(36C)	14204	8339	-712	352
H(37A)	14104	13373	-446	147
H(37B)	14961	12831	-555	147
H(38A)	15030	14631	-325	175
H(38B)	15815	14068	-519	175
H(40A)	15267	15406	-1473	207
H(40B)	16047	15153	-1134	207
H(40C)	15249	15709	-942	207
H(37C)	14410	13235	814	141
H(37D)	13850	13804	460	141
H(38C)	14787	15093	-393	152
H(38D)	14255	15545	-805	152
H(40D)	15793	13486	-1161	425
H(40E)	15050	13271	-791	425
H(40F)	15863	13851	-643	425
H(39A)	15160	14033	-1260	199
H(39B)	14365	14588	-1067	199
H(39C)	14612	14331	-1297	199
H(39D)	15428	14906	-1159	199

Table5. Torsion angles [°].

N(5)-C(1)-C(2)-C(9)	-2.9(8)
N(1)-C(1)-C(2)-C(9)	178.1(5)
N(5)-C(1)-C(2)-C(3)	178.9(4)
N(1)-C(1)-C(2)-C(3)	-0.1(5)
C(9)-C(2)-C(3)-C(16)	2.5(7)
C(1)-C(2)-C(3)-C(16)	-179.1(4)
C(9)-C(2)-C(3)-C(4)	-179.1(4)
C(1)-C(2)-C(3)-C(4)	-0.7(5)
C(16)-C(3)-C(4)-N(2)	0.2(8)
C(2)-C(3)-C(4)-N(2)	-177.9(4)
C(16)-C(3)-C(4)-N(1)	179.3(5)
C(2)-C(3)-C(4)-N(1)	1.3(5)
N(2)-C(5)-C(6)-C(7)	-173.1(4)
N(3)-C(5)-C(6)-C(7)	2.8(5)
N(2)-C(5)-C(6)-C(17)	4.2(9)
N(3)-C(5)-C(6)-C(17)	-179.8(5)
C(17)-C(6)-C(7)-C(24)	-1.4(8)
C(5)-C(6)-C(7)-C(24)	176.3(5)
C(17)-C(6)-C(7)-C(8)	179.0(5)
C(5)-C(6)-C(7)-C(8)	-3.4(5)
C(24)-C(7)-C(8)-N(4)	2.8(9)
C(6)-C(7)-C(8)-N(4)	-177.6(4)
C(24)-C(7)-C(8)-N(3)	-176.6(6)
C(6)-C(7)-C(8)-N(3)	3.0(6)
C(3)-C(2)-C(9)-O(1)	177.2(4)
C(1)-C(2)-C(9)-O(1)	-0.7(8)
C(3)-C(2)-C(9)-C(10)	-4.9(7)
C(1)-C(2)-C(9)-C(10)	177.2(5)
O(1)-C(9)-C(10)-C(15)	-177.5(4)
C(2)-C(9)-C(10)-C(15)	4.4(7)
O(1)-C(9)-C(10)-C(11)	-0.6(7)
C(2)-C(9)-C(10)-C(11)	-178.7(5)
C(15)-C(10)-C(11)-C(12)	-2.9(8)
C(9)-C(10)-C(11)-C(12)	-179.8(5)

C(10)-C(11)-C(12)-C(13)	3.0(9)
C(11)-C(12)-C(13)-C(14)	-2.6(10)
C(12)-C(13)-C(14)-C(15)	2.0(9)
C(11)-C(10)-C(15)-C(16)	-178.6(5)
C(9)-C(10)-C(15)-C(16)	-1.7(7)
C(11)-C(10)-C(15)-C(14)	2.3(8)
C(9)-C(10)-C(15)-C(14)	179.2(5)
C(13)-C(14)-C(15)-C(10)	-1.8(8)
C(13)-C(14)-C(15)-C(16)	179.1(5)
C(2)-C(3)-C(16)-O(2)	-179.0(4)
C(4)-C(3)-C(16)-O(2)	3.1(9)
C(2)-C(3)-C(16)-C(15)	0.5(7)
C(4)-C(3)-C(16)-C(15)	-177.4(5)
C(10)-C(15)-C(16)-C(3)	-0.8(8)
C(14)-C(15)-C(16)-C(3)	178.3(5)
C(10)-C(15)-C(16)-O(2)	178.7(4)
C(14)-C(15)-C(16)-O(2)	-2.2(7)
C(7)-C(6)-C(17)-O(3)	-179.4(5)
C(5)-C(6)-C(17)-O(3)	3.6(9)
C(7)-C(6)-C(17)-C(18)	2.6(7)
C(5)-C(6)-C(17)-C(18)	-174.4(5)
O(3)-C(17)-C(18)-C(19)	1.7(7)
C(6)-C(17)-C(18)-C(19)	179.9(5)
O(3)-C(17)-C(18)-C(23)	179.3(5)
C(6)-C(17)-C(18)-C(23)	-2.5(8)
C(17)-C(18)-C(19)-C(20)	-179.1(6)
C(23)-C(18)-C(19)-C(20)	3.3(9)
C(18)-C(19)-C(20)-C(21)	-4.5(10)
C(19)-C(20)-C(21)-C(22)	4.3(11)
C(20)-C(21)-C(22)-C(23)	-2.8(10)
C(19)-C(18)-C(23)-C(24)	178.9(5)
C(17)-C(18)-C(23)-C(24)	1.3(8)
C(19)-C(18)-C(23)-C(22)	-1.9(8)
C(17)-C(18)-C(23)-C(22)	-179.5(5)
C(21)-C(22)-C(23)-C(18)	1.7(8)
C(21)-C(22)-C(23)-C(24)	-179.0(6)

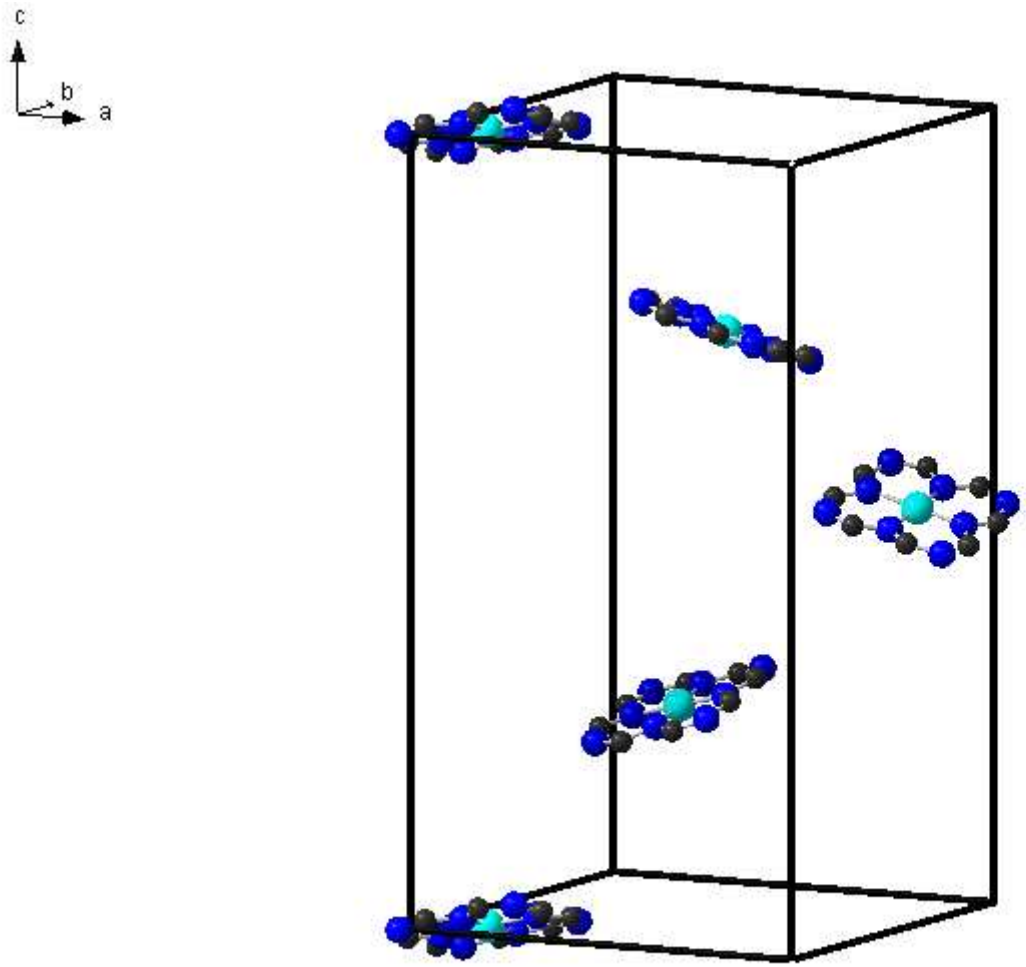
C(6)-C(7)-C(24)-O(4)	-179.4(5)
C(8)-C(7)-C(24)-O(4)	0.2(10)
C(6)-C(7)-C(24)-C(23)	0.0(8)
C(8)-C(7)-C(24)-C(23)	179.6(5)
C(18)-C(23)-C(24)-O(4)	179.5(5)
C(22)-C(23)-C(24)-O(4)	0.3(8)
C(18)-C(23)-C(24)-C(7)	0.0(8)
C(22)-C(23)-C(24)-C(7)	-179.2(5)
N(5)-C(1)-N(1)-C(4)	-178.0(4)
C(2)-C(1)-N(1)-C(4)	0.9(5)
N(5)-C(1)-N(1)-Li	8.9(6)
C(2)-C(1)-N(1)-Li	-172.2(3)
N(2)-C(4)-N(1)-C(1)	177.8(5)
C(3)-C(4)-N(1)-C(1)	-1.3(5)
N(2)-C(4)-N(1)-Li	-9.4(7)
C(3)-C(4)-N(1)-Li	171.5(3)
N(1)#1-Li-N(1)-C(1)	-3.9(3)
N(3)-Li-N(1)-C(1)	175.5(4)
N(3)#1-Li-N(1)-C(1)	-164(8)
N(1)#1-Li-N(1)-C(4)	-175.6(5)
N(3)-Li-N(1)-C(4)	3.7(4)
N(3)#1-Li-N(1)-C(4)	24(8)
N(3)-C(5)-N(2)-C(4)	11.6(7)
C(6)-C(5)-N(2)-C(4)	-173.1(5)
N(1)-C(4)-N(2)-C(5)	2.3(8)
C(3)-C(4)-N(2)-C(5)	-178.7(4)
N(4)-C(8)-N(3)-C(5)	179.4(4)
C(7)-C(8)-N(3)-C(5)	-1.3(5)
N(4)-C(8)-N(3)-Li	11.1(7)
C(7)-C(8)-N(3)-Li	-169.5(3)
N(2)-C(5)-N(3)-C(8)	174.9(5)
C(6)-C(5)-N(3)-C(8)	-0.9(5)
N(2)-C(5)-N(3)-Li	-16.5(6)
C(6)-C(5)-N(3)-Li	167.6(3)
N(1)-Li-N(3)-C(8)	174.4(4)
N(1)#1-Li-N(3)-C(8)	-26(8)

N(3)#1-Li-N(3)-C(8)	-5.0(3)
N(1)-Li-N(3)-C(5)	7.9(4)
N(1)#1-Li-N(3)-C(5)	168(8)
N(3)#1-Li-N(3)-C(5)	-171.5(4)
N(3)-C(8)-N(4)-C(8)#1	-6.0(4)
C(7)-C(8)-N(4)-C(8)#1	174.8(5)
N(1)-C(1)-N(5)-C(1)#1	-4.9(4)
C(2)-C(1)-N(5)-C(1)#1	176.3(5)
C(2)-C(9)-O(1)-C(25)	-76.2(6)
C(10)-C(9)-O(1)-C(25)	105.9(5)
C(3)-C(16)-O(2)-C(29)	87.6(6)
C(15)-C(16)-O(2)-C(29)	-91.9(5)
C(18)-C(17)-O(3)-C(33)	-123.5(5)
C(6)-C(17)-O(3)-C(33)	58.5(7)
C(7)-C(24)-O(4)-C(37A)	71.2(8)
C(23)-C(24)-O(4)-C(37A)	-108.2(8)
C(7)-C(24)-O(4)-C(37)	-74.1(8)
C(23)-C(24)-O(4)-C(37)	106.4(7)
C(9)-O(1)-C(25)-C(26)	-163.4(6)
O(1)-C(25)-C(26)-C(27)	55.5(9)
C(25)-C(26)-C(27)-C(28)	-178.1(8)
C(16)-O(2)-C(29)-C(30)	-176.3(4)
O(2)-C(29)-C(30)-C(31)	-65.3(6)
C(29)-C(30)-C(31)-C(32)	-175.6(5)
C(17)-O(3)-C(33)-C(34)	139.1(7)
O(3)-C(33)-C(34)-C(35)	171.3(7)
C(33)-C(34)-C(35)-C(36)	65.7(12)
C(24)-O(4)-C(37)-C(38)	-153.1(9)
C(37A)-O(4)-C(37)-C(38)	69.6(13)
O(4)-C(37)-C(38)-C(39)	-170.3(10)
C(24)-O(4)-C(37A)-C(38A)#1	139.2(9)
C(37)-O(4)-C(37A)-C(38A)#1	-82.7(12)
C(37)-C(38)-C(39)-C(40)	179.3(12)
C(37)-C(38)-C(39)-C(40A)	-69(2)
C(37)-C(38)-C(39)-C(38A)	98.0(13)
C(37A)#1-C(38A)-C(39)-C(40)	162.0(11)

C(37A)#1-C(38A)-C(39)-C(40A)	-70(2)
C(37A)#1-C(38A)-C(39)-C(38)	-81.7(10)

Symmetry transformations used to generate equivalent atoms:
#1 y,x,-z

Supplement –B



Unit cell packing of diagram for tetragonal form of LiNc-BuO (T_d) with only the Li, C, N atoms and the core of the molecule. This shows the lack of stacking between the central cores.