Electronic Supplementary Information

Access to unusual fluorenone and pyridyl ketone substitution patterns via sodium alkylamidozincate intermediates

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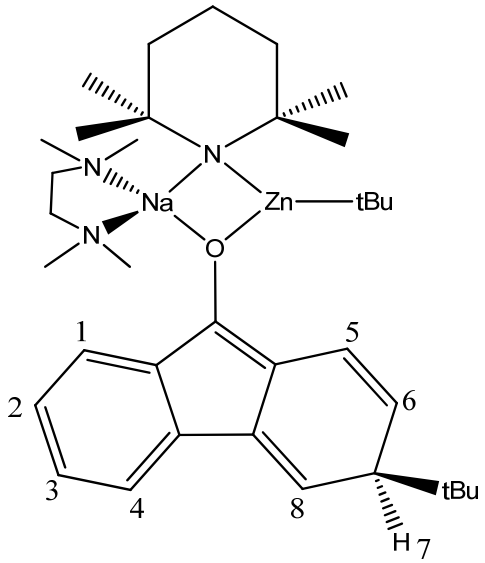
Synthesis of [(TMEDA)·Na(μ-$OC_{13}H_8$-3-^{t}Bu)(μ-TMP)Zn(^{t}Bu)] (**2**): A solution of ^{t}Bu_2Zn (0.36 g, 2 mmol) in hexane (10 mL) was transferred by cannula to a suspension of NaTMP in hexane [prepared *in situ* by reaction of ^{n}BuNa (0.16 g, 2 mmol) with TMP(H) (0.34 mL, 2 mmol)]. TMEDA (0.30 mL, 2 mmol) was then added. The resultant suspension was gently heated to produce a homogenous yellow solution to yield an *in situ* mixture of **1**. Fluorenone (0.36 g, 2 mmol) was added to the solution and the reaction mixture was allowed to stir at ambient temperature for 30 minutes. The resulting deep red solution was placed in a freezer (−28°C). Large yellow crystals of **2** were formed after 24 hours (0.842 g, 66 %).



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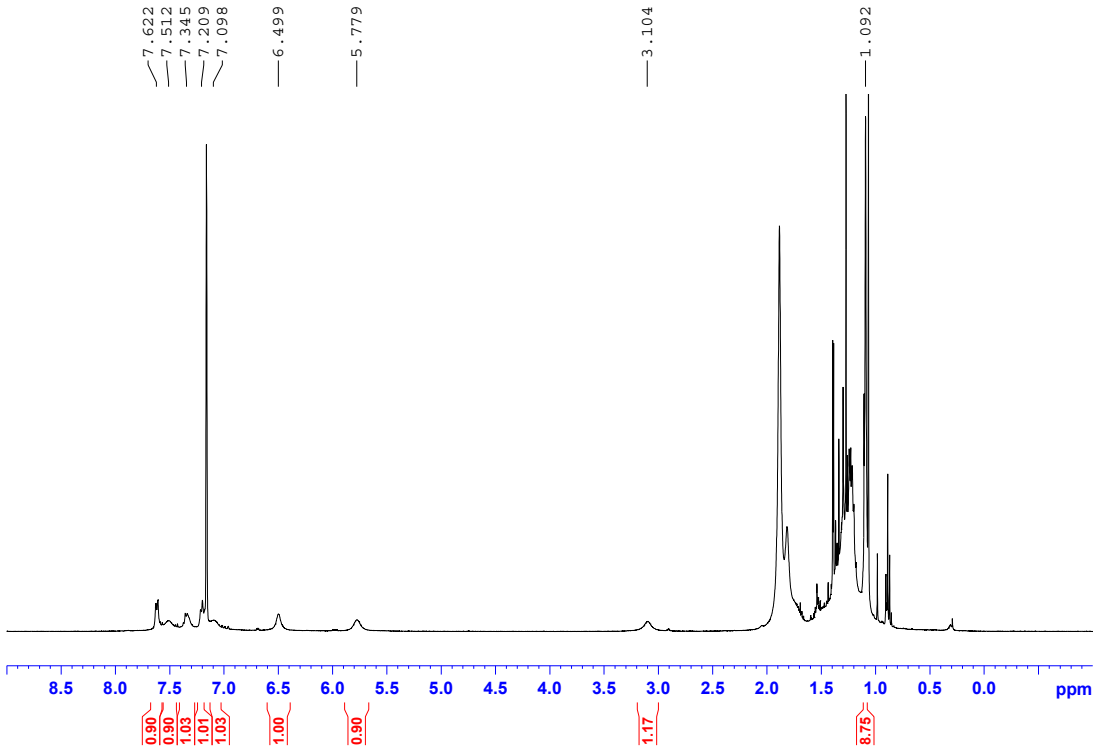
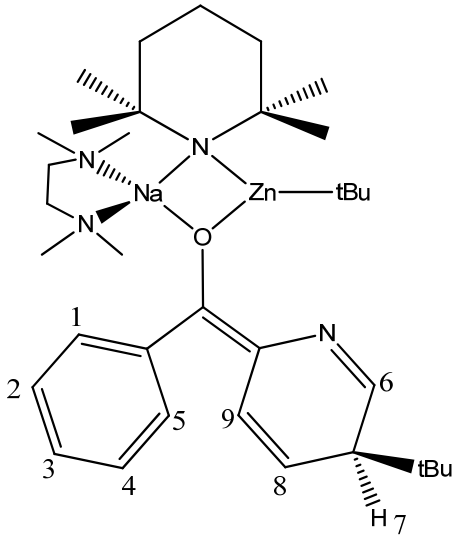


^{1}H NMR (400.13 MHz, 298K, C_6D_6):- δ 7.66 (1H, bd, C_1), 7.51 (1H, bd, C_4), 7.34 (1H, bt, C_2), 7.21 (1H, bt, C_3), 7.10 (1H, bs, C_5), 6.50 (1H, bs, C_8), 5.78 (1H, bs, C_6), 3.10 (1H, bs, C_7), 1.87 (12H, s, TMEDA-CH_3), 1.80 (4H, s, TMEDA-CH_2), 1.09 (9H, s, ^{t}Bu)

^{13}C NMR:- δ 127.0 (C_3), 124.7 (C_4), 122.3 (C_5), 119.9 (C_6), 118.8 (C_2), 117.1 (C_5), 116.7 (C_8), 57.1 (TMEDA-CH_2), 47.3 (TMEDA-CH_3), 50.7 (C_7), 27.1 (^{t}Bu)



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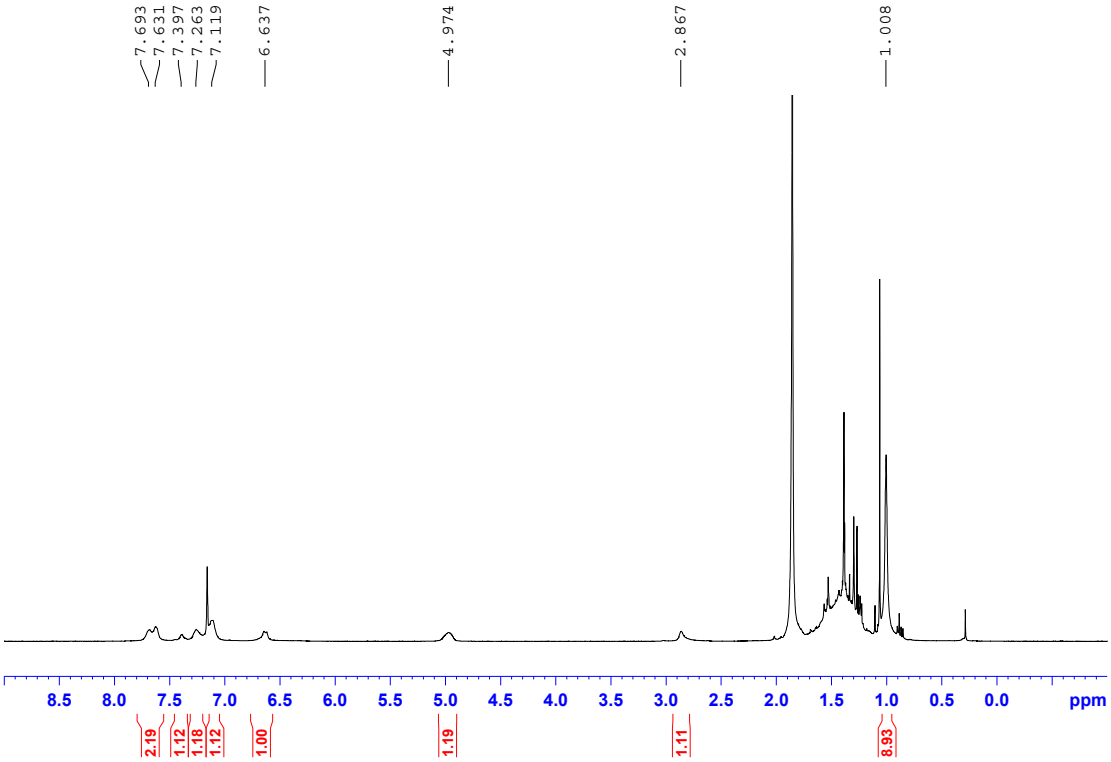
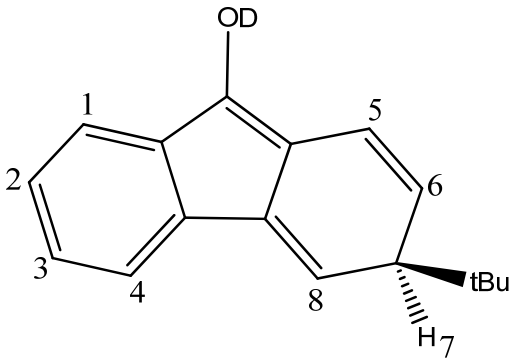
Synthesis of [(TMEDA)·Na{μ-O(Ph)-2-C_5H_4N-4-^{t}Bu)(μ-TMP)Zn(^{t}Bu)] (**3**): A solution of $^t Bu_2Zn$ (0.36 g, 2 mmol) in hexane (10 mL) was transferred by cannula to a suspension of NaTMP in hexane [prepared *in situ* by reaction of ^{n}BuNa (0.16 g, 2 mmol) with TMP(H) (0.34 mL, 2 mmol)]. TMEDA (0.30 mL, 2 mmol) was then added. The resultant suspension was gently heated to produce a homogenous yellow solution to yield an *in situ* mixture of **1**. 2-Benzoylpyridine (0.366 g, 2 mmol) was added to the solution and the reaction mixture was allowed to stir at ambient temperature for 30 minutes. The resulting green solution was placed in a freezer (−28°C). Yellow crystals of **3** were formed after 24 hours (0.716 g, 56 %).

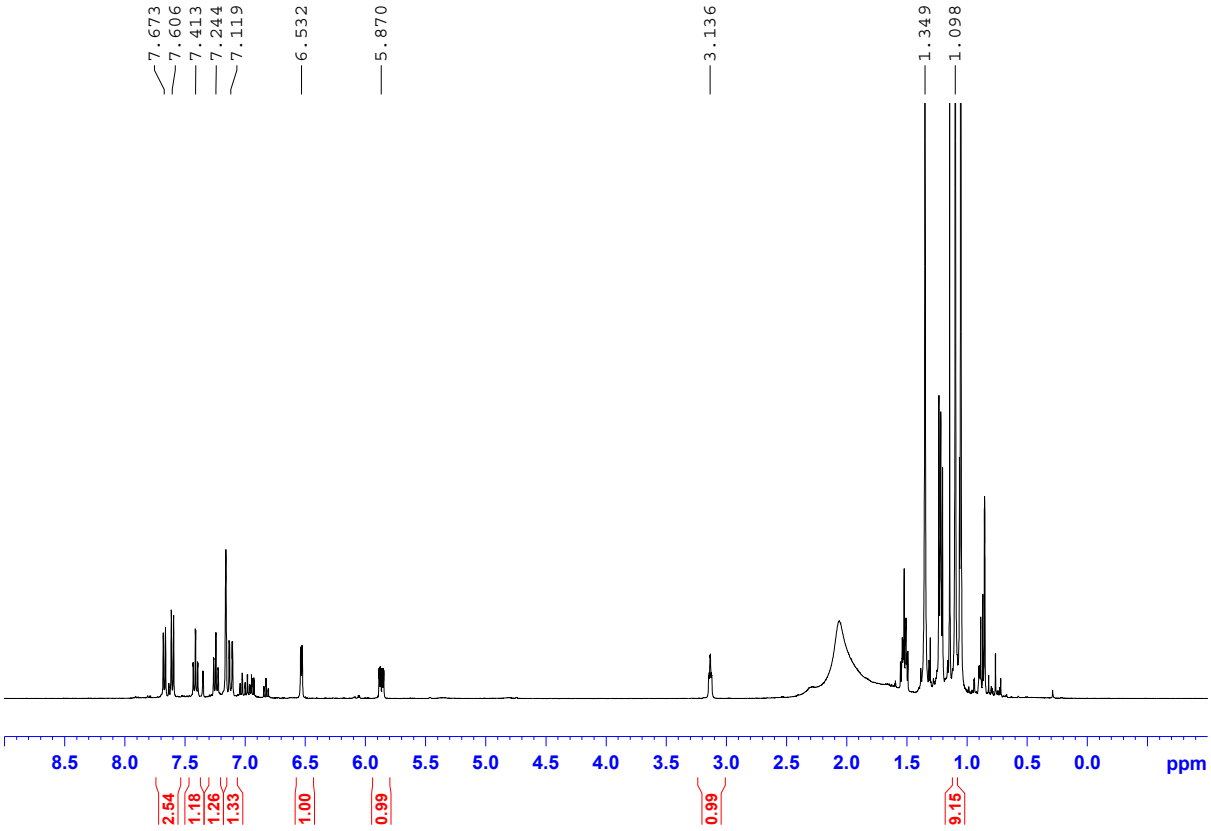


^{1}H NMR (400.13 MHz, 298K, C_6D_6):- δ 7.69 (1H, bs, C_2), 7.65 (1H, bs, C_4), 7.39 (1H, bs, C_6), 7.26 (1H, bs, C_3), 7.12 (2H, bs, $C_{1/5}$), 6.64 (1H, bs, C_9), 4.97 (1H, bs, C_8), 2.87 (1H, bs, C_7), 1.90 (16H, bs, TMEDA), 1.01 (9H, s, ^{t}Bu), 1.07 [12H, TMP (α-CH_3)], 1.38 [4H, TMP (β-CH_2)]

^{13}C NMR :- δ 128.5 (2H, C_2/C_4), 149.9 (C_6), 126.9 (C_3), 126.7 (2H, C_1/C_5), 125.6 (C_9), 109.3(C_8), 49.5 (C_7), 33.3 [4H, TMP(H)(β-CH_2)], 31.1 [12H, TMP(H)(α-CH_3)], 1.01 (9H,(^{t}Bu))

Electronic Supplementary Information

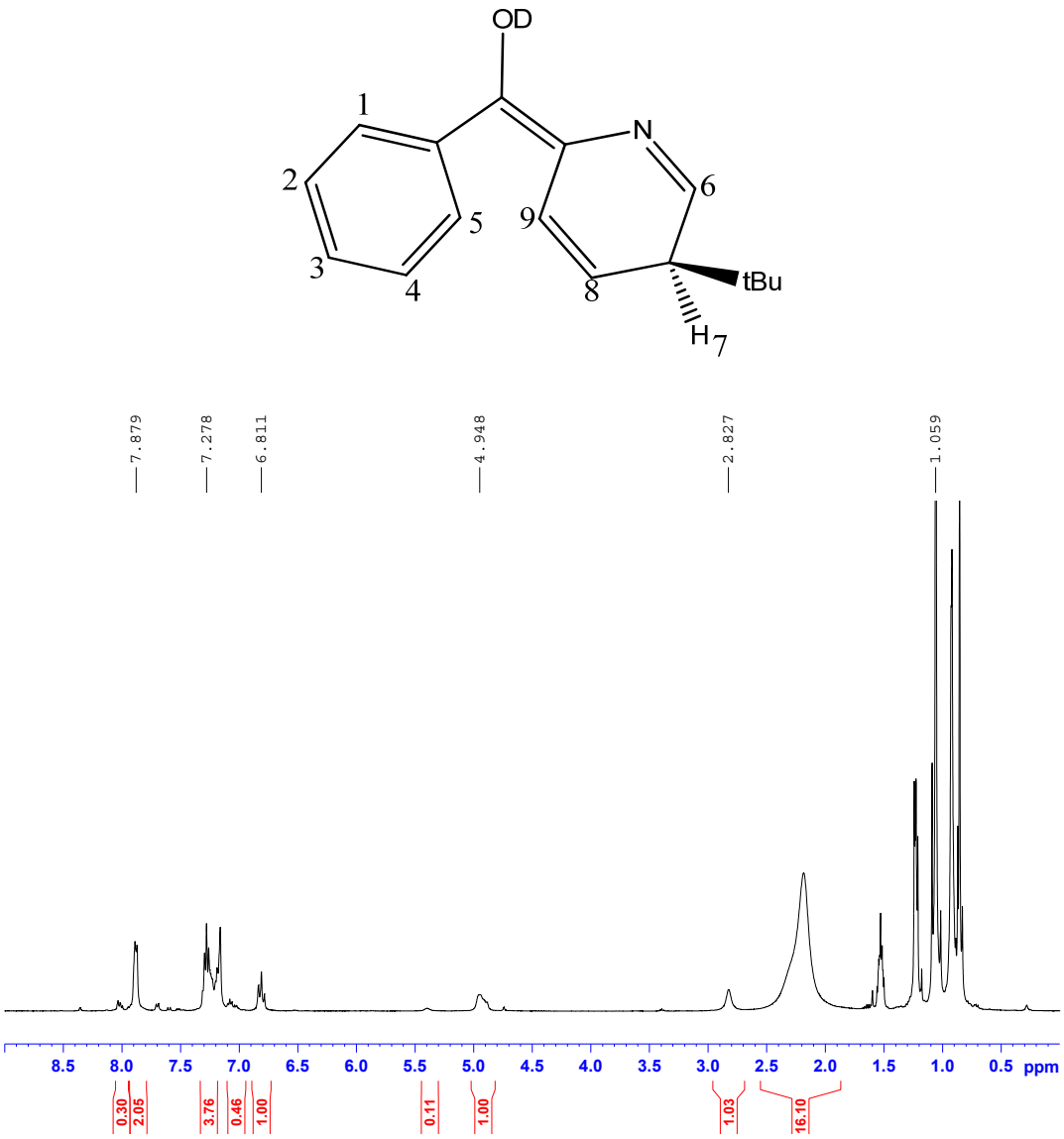




^{1}H NMR (400.13 MHz, 298K, C_6D_6):- δ 7.67 (2H, bd, C_1), 7.61 (4H, bd, C_4), 7.41 (1H, bt, C_2), 7.24 (1H, bt, C_3), 7.12 (1H, bs, C_5), 6.53 (1H, bs, C_8), 5.87 (1H, bs, C_6), 3.14 (1H, bs, C_7), 2.07 (16H, TMEDA), 1.35 (9H, iso-butane), 1.22 [4H, TMP(H)(β-CH_2)], 1.10 (9H, s, ^{t}Bu), 1.05 [12H, TMP(H)(α-CH_3)]

^{13}C NMR :- δ 126.7 (C_2), 124.6 (C_3), 123.3 (C_5), 118.8 (C_1), 118.7 (C_6),117.8 (C_4), 115.5 (C_8), 50.9 (C_7), 47.1 (TMEDA-CH_3), 45.8 (TMEDA-CH_2), 38.4 [TMP(H)(β-CH_2), 34.8 (iso-butane), 31.7 [TMP(H)(α-CH_3), 27.9 (^{t}Bu)

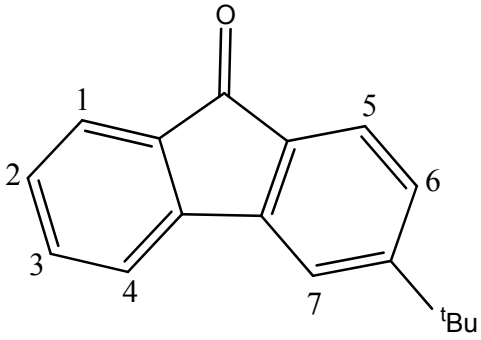
Electronic Supplementary Information

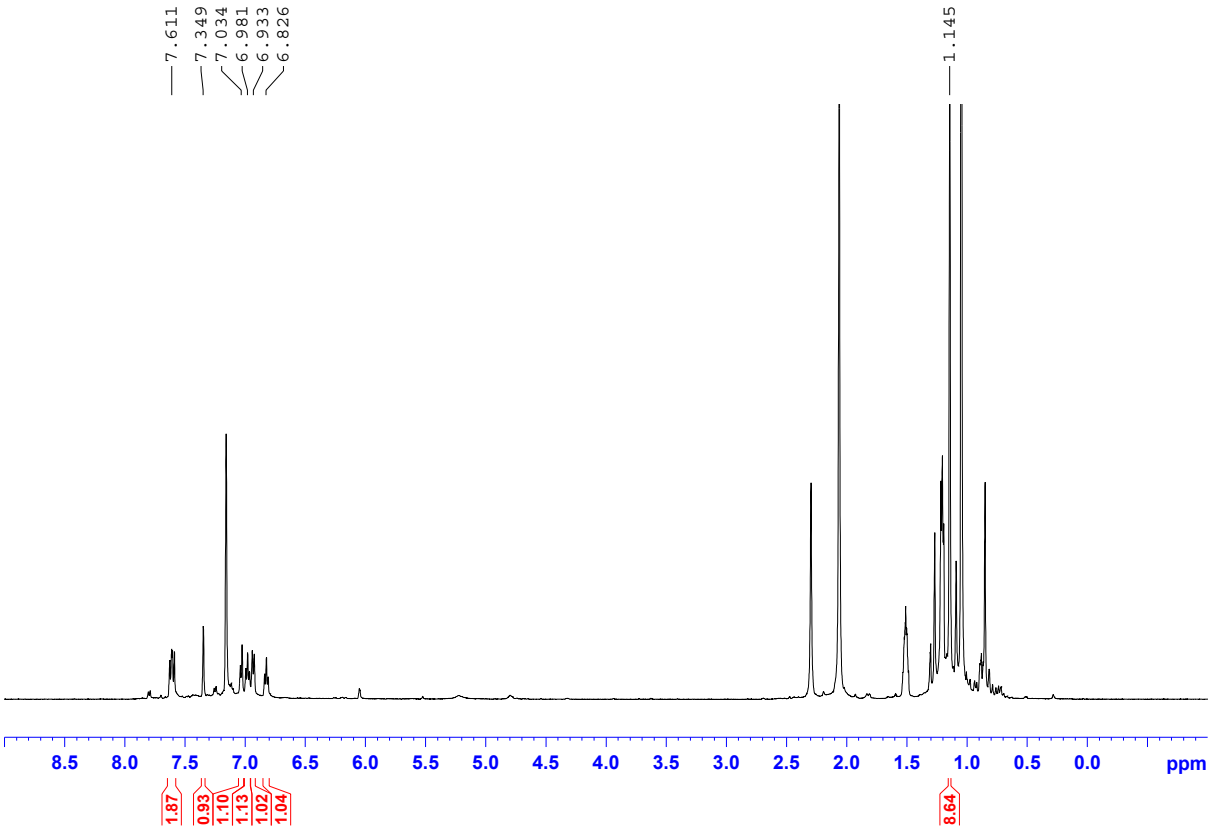


^{1}H NMR (400.13 MHz, 298K, C_6D_6):- δ 7.88 (2H, bs, $C_{2/4}$), 7.28 (4H, bs, $C_{1/5/3,6}$),7.16 (1H, bd, C_9) 4.95 (1H, bs, C_8), 2.83 (1H, bs, C_7), 2.19 (16H, bs, TMEDA), 1.53 [2H,TMP(H)(γ-CH_2)], 1.22 [4H, TMP(H)(β-CH_2)], 1.06 [12H, TMP(H)(α-CH_3)], 0.92 (9H, ^{t}Bu)

^{13}C NMR :- δ 148.7 ($C_{1/5/3,6}$), 129.1 ($C_{2/4}$), 127.8 (C_9), 127.5 (C1?), 126.0 (?), 109.5 (C_8), 50.0 (C_7), 46.0 (TMEDA), 38.6 [TMP(H)(β-CH_2)], 31.9 [TMP(H)(α-CH_3)], 26.8 (^{t}Bu), 18.8 [TMP(H)(γ-CH_2)]

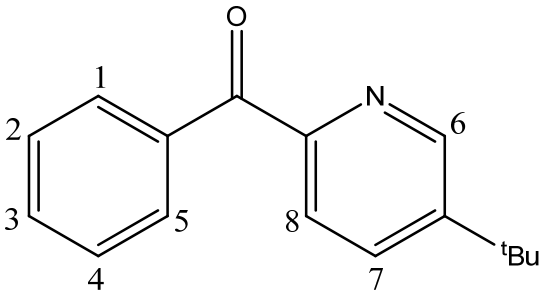
Electronic Supplementary Information

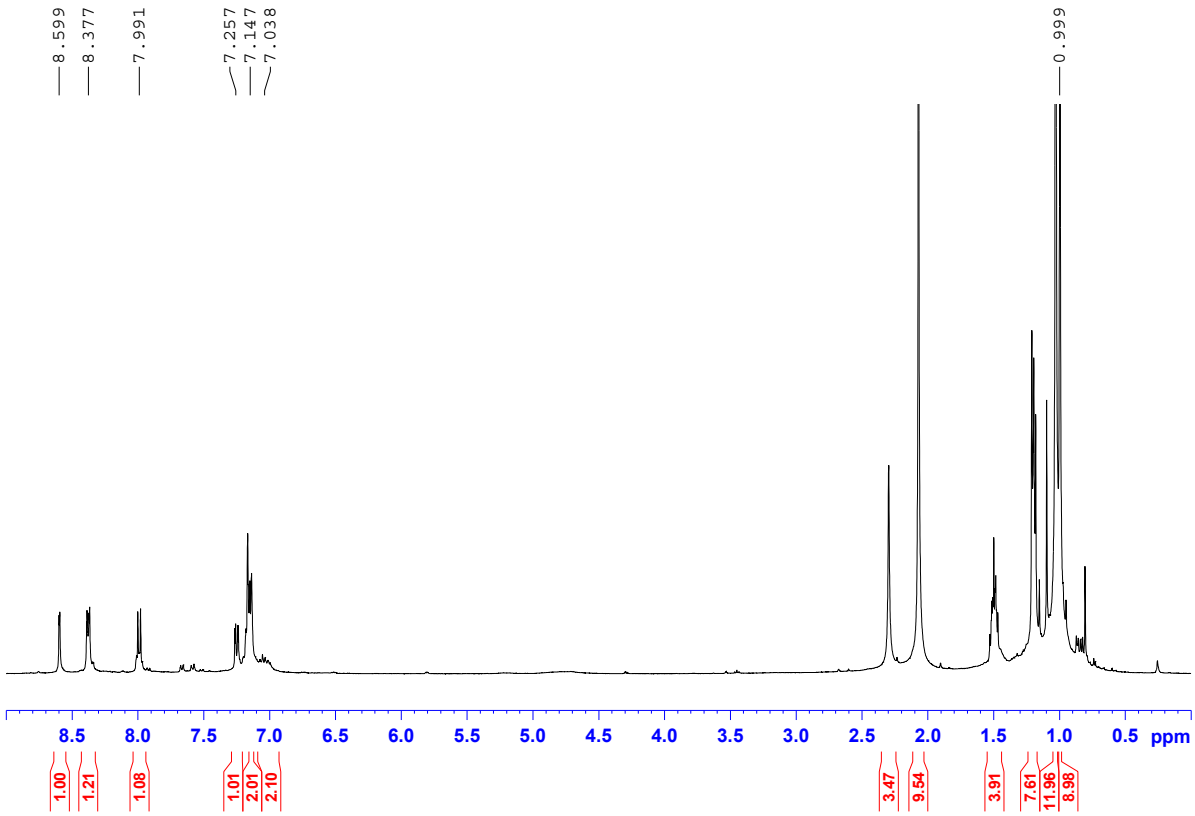




^{1}H NMR (400.13 MHz, 298K, C_6D_6):- 7.61 (2H, d, $C_{1/4}$), 7.35 (1H, s, C_7), 7.03 (1H, d, C_5), 6.98 (1H, t, C_2), 6.93 (1H, d, C_6) 6.83 (1H, t, C_3), 2.30 (TMEDA-CH_2), 2.06 (TMEDA-CH_3), 1.51 [2H, TMP(H)(γ-CH_2)], 1.21 [4H, TMP(H)(β-CH_2)], 1.15 (9H, ^{t}Bu), 1.05 [TMP(H)(α-CH_3)]

Electronic Supplementary Information





^{1}H NMR (400.13 MHz, 298K, C_6D_6):- 8.60 (1H, s, C_6), 8.38 (1H, d, C_1), 7.99 (1H, d, C_5), 7.25 (1H, m, C_3), 7.14 (2H, t, $C_{2/4}$), 7.06 (1H, d, C_7), 6.99 (1H, d, C_8), 2.30 (TMEDA-CH_2), 2.07 (TMEDA-CH_3), 1.50 [2H, TMP(H)(γ-CH_2)], 1.20 [4H, TMP(H)(β-CH_2)],1.30 [TMP(H)(α-CH_3)], 0.99 (^{t}Bu)

^{13}C NMR :- δ 146.1 (C_6), 133.8(C_3), 131.6 (C_1), 128.1 (C_8), 127.9 ($C_{2/4}$), 126.8 (C_7), 124.3 (C_5), 58.2 (TMEDA-CH_2), 45.8 (TMEDA-CH_3), 31.8 [TMP(H)(α-CH_3)], 30.6 (^{t}Bu), 27.2 [TMP(H)(β-CH_2)], 18.7 [TMP(H)(β-CH_2)]

Selected bond distances (Å) and angles (°) for **2** : Na1–N3, 2.442(3); Na1–O2, 2.242(2); Zn1–N3, 1.952(2); Zn1–C1, 1.994(3); Zn1–O2, 2.018(2); Na1–N3–Zn1, 90.19(10); N3–Zn1–O2, 96.75(9); Zn1–O2–Na1, 94.49(9); N41–Na1–N44, 75.45(9); N41–Na1–N3, 133.52(11); N41–Na1–O2, 106.52(10); N44–Na1–N3, 141.70(10); N44–Na1–O2, 122.03(9); N3–Zn1–C1, 148.43(12); O2–Zn1–C1 114.79(11).

Full X-ray data for **2**

Table 1. Crystal data and structure refinement for jksamboth.

Identification code	jkcben11	
Empirical formula	C36 H60 N3 Na O Zn	
Formula weight	639.23	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 10.2426(6) Å	α= 90°.
	b = 19.6573(15) Å	β= 94.903(6)°.
	c = 36.846(3) Å	γ = 90°.
Volume	7391.5(9) Å^3	
Z	8	
Density (calculated)	1.149 Mg/m^3	
Absorption coefficient	0.706 mm^{-1}	
F(000)	2768	
Crystal size	0.3 x 0.1 x 0.06 mm^3	
Theta range for data collection	3.14 to 26.00°.	
Index ranges	-11<=h<=12, -24<=k<=24, -45<=l<=45	
Reflections collected	49503	
Independent reflections	14502 [R(int) = 0.0842]	
Completeness to theta = 26.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.50172	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14502 / 49 / 786	
Goodness-of-fit on F^2	0.762	
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.0801	
R indices (all data)	R1 = 0.1366, wR2 = 0.0910	
Largest diff. peak and hole	0.502 and -0.620 e.Å^{-3}	

Electronic Supplementary Information

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

	x	y	z	U(eq)
Na(1)	3749(1)	4816(1)	1658(1)	31(1)
Zn(1)	1275(1)	5655(1)	1829(1)	27(1)
Na(2)	1854(1)	5326(1)	6194(1)	33(1)
Zn(2)	4272(1)	4488(1)	5994(1)	41(1)
C(1)	-597(3)	5913(2)	1855(1)	31(1)
C(11)	-1375(3)	5302(2)	1968(1)	59(1)
C(12)	-1185(3)	6157(2)	1482(1)	48(1)
C(13)	-727(3)	6487(2)	2129(1)	45(1)
O(2)	1558(2)	4739(1)	1601(1)	31(1)
C(21)	689(3)	4290(2)	1470(1)	27(1)
C(22)	-9(3)	4261(2)	1134(1)	32(1)
C(23)	-163(3)	4731(2)	833(1)	44(1)
C(24)	-940(3)	4582(2)	528(1)	48(1)
C(25)	-1603(3)	3895(2)	461(1)	47(1)
C(26)	-1573(3)	3483(2)	809(1)	41(1)
C(27)	-810(3)	3650(2)	1108(1)	30(1)
C(28)	-602(3)	3304(2)	1462(1)	25(1)
C(29)	-1112(3)	2714(2)	1599(1)	29(1)
C(210)	-743(3)	2530(2)	1957(1)	37(1)
C(211)	125(3)	2926(2)	2171(1)	38(1)
C(212)	654(3)	3508(2)	2036(1)	32(1)
C(213)	303(3)	3697(2)	1683(1)	24(1)
C(20)	-1000(4)	3498(2)	154(1)	51(1)
C(214)	490(4)	3421(2)	254(1)	82(2)
C(215)	-1215(4)	3871(2)	-208(1)	76(1)
C(216)	-1630(4)	2791(2)	110(1)	75(1)
N(3)	3123(2)	5879(1)	1940(1)	25(1)
C(31)	3581(3)	6455(2)	1719(1)	28(1)
C(311)	2762(3)	6443(2)	1355(1)	40(1)
C(312)	5033(3)	6378(2)	1641(1)	38(1)
C(32)	3398(3)	7144(2)	1901(1)	45(1)
C(33)	3960(4)	7162(2)	2293(1)	58(1)
C(34)	3344(3)	6598(2)	2504(1)	49(1)

Electronic Supplementary Information

C(35)	3514(3)	5894(2)	2338(1)	30(1)
C(351)	2619(3)	5402(2)	2519(1)	44(1)
C(352)	4930(3)	5641(2)	2436(1)	47(1)
N(41)	4491(3)	4533(2)	1061(1)	38(1)
C(411)	5587(4)	4911(2)	942(1)	71(1)
C(412)	3345(4)	4615(2)	791(1)	72(1)
C(42)	4831(3)	3813(2)	1099(1)	43(1)
C(43)	5723(3)	3651(2)	1427(1)	44(1)
N(44)	5188(2)	3792(1)	1775(1)	28(1)
C(441)	4247(3)	3262(2)	1856(1)	50(1)
C(442)	6251(3)	3798(2)	2063(1)	41(1)
C(5)	6117(6)	4259(3)	5893(2)	40(1)
C(51)	7055(4)	4582(3)	6184(2)	59(2)
C(52)	6266(15)	3477(4)	5912(5)	63(3)
C(53)	6447(5)	4519(4)	5522(2)	59(2)
O(6)	3974(2)	5469(1)	6124(1)	39(1)
C(61)	4829(3)	5975(2)	6150(1)	32(1)
C(62)	5236(3)	6384(2)	5880(1)	34(1)
C(63)	4981(4)	6393(2)	5492(1)	54(1)
C(64)	5550(4)	6843(2)	5290(1)	57(1)
C(65)	6471(4)	7403(2)	5438(1)	47(1)
C(66)	6764(3)	7339(2)	5845(1)	43(1)
C(67)	6165(3)	6883(2)	6043(1)	35(1)
C(68)	6299(3)	6753(2)	6437(1)	27(1)
C(69)	7026(3)	7067(2)	6724(1)	31(1)
C(610)	6949(3)	6814(2)	7071(1)	35(1)
C(611)	6180(3)	6254(2)	7128(1)	38(1)
C(612)	5446(3)	5941(2)	6843(1)	33(1)
C(613)	5492(3)	6197(2)	6498(1)	27(1)
C(60)	5989(4)	8119(2)	5330(1)	44(1)
C(614)	4720(3)	8265(2)	5516(1)	66(1)
C(615)	5708(4)	8169(2)	4917(1)	62(1)
C(616)	6997(3)	8658(2)	5450(1)	53(1)
N(7)	2376(9)	4202(5)	6033(2)	23(2)
C(71)	1857(5)	3940(3)	5675(2)	29(2)
C(711)	2449(5)	4368(3)	5376(1)	39(2)
C(712)	364(7)	4095(6)	5596(3)	54(2)
C(72)	2184(5)	3185(2)	5611(2)	37(1)

Electronic Supplementary Information

C(73)	1846(5)	2755(3)	5913(1)	42(2)
C(74)	2485(6)	3008(3)	6287(2)	51(2)
C(75)	2184(5)	3758(3)	6356(2)	37(2)
C(751)	814(5)	3827(3)	6477(2)	45(2)
C(752)	3051(6)	4020(4)	6678(2)	53(2)
N(7A)	2600(20)	4220(12)	5947(3)	23(2)
C(100)	1851(10)	4129(5)	5586(3)	26(4)
C(101)	366(12)	4011(11)	5619(6)	33
C(102)	139(9)	3521(5)	5918(3)	36
C(103)	852(10)	3661(8)	6298(3)	74(5)
C(104)	2328(9)	3720(5)	6238(3)	32(4)
C(105)	2286(12)	3493(6)	5392(4)	82(5)
C(106)	2145(14)	4755(6)	5365(4)	69(4)
C(107)	3272(13)	3907(8)	6576(4)	53(2)
C(108)	2763(8)	2990(2)	6142(1)	78(6)
N(81)	586(3)	6292(1)	5945(1)	47(1)
C(811)	1616(3)	6752(1)	5845(1)	83(2)
C(812)	-343(4)	6200(3)	5630(1)	99(2)
C(82)	-97(4)	6569(2)	6245(1)	68(1)
C(83)	573(4)	6511(2)	6605(1)	73(1)
N(84)	866(3)	5817(2)	6737(1)	42(1)
C(841)	-283(4)	5490(2)	6853(1)	85(2)
C(842)	1842(3)	5878(2)	7050(1)	71(1)
C(5A)	6072(12)	4153(7)	6007(3)	40(1)
C(51A)	6609(15)	4631(8)	5728(4)	82(6)
C(52A)	6853(14)	4208(8)	6373(3)	81(6)
C(53A)	6350(40)	3471(11)	5829(10)	77(10)

Table 3. Bond lengths [Å] and angles [°] for jksamboth.

Na(1)-O(2)	2.242(2)
Na(1)-N(3)	2.442(3)
Na(1)-N(41)	2.453(3)
Na(1)-N(44)	2.511(3)
Na(1)-C(42)	3.125(4)
Na(1)-Zn(1)	3.1314(11)
Zn(1)-N(3)	1.952(2)
Zn(1)-C(1)	1.994(3)
Zn(1)-O(2)	2.018(2)
Na(2)-O(6)	2.227(2)
Na(2)-N(7)	2.361(11)
Na(2)-N(81)	2.436(3)
Na(2)-N(7A)	2.50(3)
Na(2)-N(84)	2.510(3)
Na(2)-Zn(2)	3.1140(12)
Na(2)-C(83)	3.128(4)
Zn(2)-N(7A)	1.786(18)
Zn(2)-C(5A)	1.955(14)
Zn(2)-C(5)	2.009(7)
Zn(2)-O(6)	2.016(2)
Zn(2)-N(7)	2.038(8)
C(1)-C(11)	1.519(4)
C(1)-C(13)	1.528(4)
C(1)-C(12)	1.531(4)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
O(2)-C(21)	1.316(3)
C(21)-C(22)	1.375(4)
C(21)-C(213)	1.478(4)

Electronic Supplementary Information

C(22)-C(23)	1.442(4)
C(22)-C(27)	1.453(4)
C(23)-C(24)	1.353(4)
C(23)-H(63A)	0.9500
C(24)-C(25)	1.523(5)
C(24)-H(64A)	0.9500
C(25)-C(26)	1.516(5)
C(25)-C(20)	1.545(5)
C(25)-H(25A)	1.0000
C(26)-C(27)	1.335(4)
C(26)-H(66A)	0.9500
C(27)-C(28)	1.473(4)
C(28)-C(29)	1.384(4)
C(28)-C(213)	1.410(4)
C(29)-C(210)	1.386(4)
C(29)-H(69A)	0.9500
C(210)-C(211)	1.378(4)
C(210)-H(61J)	0.9500
C(211)-C(212)	1.377(4)
C(211)-H(61K)	0.9500
C(212)-C(213)	1.372(4)
C(212)-H(61L)	0.9500
C(20)-C(215)	1.521(5)
C(20)-C(216)	1.536(5)
C(20)-C(214)	1.547(5)
C(214)-H(61G)	0.9800
C(214)-H(61H)	0.9800
C(214)-H(61I)	0.9800
C(215)-H(61D)	0.9800
C(215)-H(61E)	0.9800
C(215)-H(61F)	0.9800
C(216)-H(61A)	0.9800
C(216)-H(61B)	0.9800
C(216)-H(61C)	0.9800
N(3)-C(35)	1.485(4)
N(3)-C(31)	1.496(4)
C(31)-C(311)	1.520(4)
C(31)-C(32)	1.530(4)

Electronic Supplementary Information

C(31)-C(312)	1.545(4)
C(311)-H(71A)	0.9800
C(311)-H(71B)	0.9800
C(311)-H(71C)	0.9800
C(312)-H(71D)	0.9800
C(312)-H(71E)	0.9800
C(312)-H(71F)	0.9800
C(32)-C(33)	1.509(5)
C(32)-H(72A)	0.9900
C(32)-H(72B)	0.9900
C(33)-C(34)	1.522(5)
C(33)-H(73A)	0.9900
C(33)-H(73B)	0.9900
C(34)-C(35)	1.529(4)
C(34)-H(74A)	0.9900
C(34)-H(74B)	0.9900
C(35)-C(351)	1.526(4)
C(35)-C(352)	1.547(4)
C(351)-H(75A)	0.9800
C(351)-H(75B)	0.9800
C(351)-H(75C)	0.9800
C(352)-H(75D)	0.9800
C(352)-H(75E)	0.9800
C(352)-H(75F)	0.9800
N(41)-C(411)	1.445(4)
N(41)-C(42)	1.462(4)
N(41)-C(412)	1.480(4)
C(411)-H(81A)	0.9800
C(411)-H(81B)	0.9800
C(411)-H(81C)	0.9800
C(412)-H(81D)	0.9800
C(412)-H(81E)	0.9800
C(412)-H(81F)	0.9800
C(42)-C(43)	1.487(4)
C(42)-H(82A)	0.9900
C(42)-H(82B)	0.9900
C(43)-N(44)	1.463(4)
C(43)-H(83A)	0.9900

Electronic Supplementary Information

C(43)-H(83B)	0.9900
N(44)-C(442)	1.454(4)
N(44)-C(441)	1.467(4)
C(441)-H(84A)	0.9800
C(441)-H(84B)	0.9800
C(441)-H(84C)	0.9800
C(442)-H(84D)	0.9800
C(442)-H(84E)	0.9800
C(442)-H(84F)	0.9800
C(5)-C(51)	1.516(6)
C(5)-C(53)	1.524(6)
C(5)-C(52)	1.546(8)
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
O(6)-C(61)	1.323(4)
C(61)-C(62)	1.371(5)
C(61)-C(613)	1.466(4)
C(62)-C(63)	1.431(5)
C(62)-C(67)	1.461(4)
C(63)-C(64)	1.323(5)
C(63)-H(23A)	0.9500
C(64)-C(65)	1.520(5)
C(64)-H(24A)	0.9500
C(65)-C(66)	1.508(5)
C(65)-C(60)	1.533(5)
C(65)-H(65A)	1.0000
C(66)-C(67)	1.336(4)
C(66)-H(26A)	0.9500
C(67)-C(68)	1.469(4)
C(68)-C(69)	1.384(4)
C(68)-C(613)	1.400(4)

Electronic Supplementary Information

C(69)-C(610)	1.383(4)
C(69)-H(29A)	0.9500
C(610)-C(611)	1.380(4)
C(610)-H(21J)	0.9500
C(611)-C(612)	1.383(4)
C(611)-H(21K)	0.9500
C(612)-C(613)	1.369(4)
C(612)-H(21L)	0.9500
C(60)-C(616)	1.521(5)
C(60)-C(615)	1.527(4)
C(60)-C(614)	1.547(4)
C(614)-H(21A)	0.9800
C(614)-H(21B)	0.9800
C(614)-H(21C)	0.9800
C(615)-H(21D)	0.9800
C(615)-H(21E)	0.9800
C(615)-H(21F)	0.9800
C(616)-H(21G)	0.9800
C(616)-H(21H)	0.9800
C(616)-H(21I)	0.9800
N(7)-C(71)	1.473(6)
N(7)-C(75)	1.503(6)
C(71)-C(72)	1.543(6)
C(71)-C(711)	1.552(6)
C(71)-C(712)	1.562(6)
C(711)-H(31A)	0.9800
C(711)-H(31B)	0.9800
C(711)-H(31C)	0.9800
C(712)-H(31D)	0.9800
C(712)-H(31E)	0.9800
C(712)-H(31F)	0.9800
C(72)-C(73)	1.463(5)
C(72)-H(32A)	0.9900
C(72)-H(32B)	0.9900
C(73)-C(74)	1.556(6)
C(73)-H(33A)	0.9900
C(73)-H(33B)	0.9900
C(74)-C(75)	1.533(6)

Electronic Supplementary Information

C(74)-H(34A)	0.9900
C(74)-H(34B)	0.9900
C(75)-C(752)	1.509(6)
C(75)-C(751)	1.513(6)
C(751)-H(35A)	0.9800
C(751)-H(35B)	0.9800
C(751)-H(35C)	0.9800
C(752)-H(35D)	0.9800
C(752)-H(35E)	0.9800
C(752)-H(35F)	0.9800
N(7A)-C(100)	1.488(9)
N(7A)-C(104)	1.499(9)
C(100)-C(106)	1.520(9)
C(100)-C(105)	1.526(9)
C(100)-C(101)	1.553(9)
C(101)-C(102)	1.498(10)
C(101)-H(10A)	0.9900
C(101)-H(10B)	0.9900
C(102)-C(103)	1.548(9)
C(102)-H(10C)	0.9900
C(102)-H(10D)	0.9900
C(103)-C(104)	1.550(9)
C(103)-H(10E)	0.9900
C(103)-H(10F)	0.9900
C(104)-C(107)	1.552(9)
C(104)-C(108)	1.554(8)
C(105)-H(10G)	0.9800
C(105)-H(10H)	0.9800
C(105)-H(10I)	0.9800
C(106)-H(10J)	0.9800
C(106)-H(10K)	0.9800
C(106)-H(10L)	0.9800
C(107)-H(10M)	0.9800
C(107)-H(10N)	0.9800
C(107)-H(10O)	0.9800
C(108)-H(10P)	0.9800
C(108)-H(10Q)	0.9800
C(108)-H(10R)	0.9800

Electronic Supplementary Information

N(81)-C(812)	1.446(4)
N(81)-C(811)	1.460(2)
N(81)-C(82)	1.463(4)
C(811)-H(41A)	0.9799
C(811)-H(41B)	0.9800
C(811)-H(41C)	0.9798
C(812)-H(41D)	0.9800
C(812)-H(41E)	0.9800
C(812)-H(41F)	0.9800
C(82)-C(83)	1.445(5)
C(82)-H(42A)	0.9900
C(82)-H(42B)	0.9900
C(83)-N(84)	1.470(5)
C(83)-H(43A)	0.9900
C(83)-H(43B)	0.9900
N(84)-C(841)	1.438(4)
N(84)-C(842)	1.465(4)
C(841)-H(44A)	0.9800
C(841)-H(44B)	0.9800
C(841)-H(44C)	0.9800
C(842)-H(44D)	0.9800
C(842)-H(44E)	0.9800
C(842)-H(44F)	0.9800
C(5A)-C(52A)	1.510(9)
C(5A)-C(53A)	1.530(10)
C(5A)-C(51A)	1.531(9)
C(51A)-H(51D)	0.9800
C(51A)-H(51E)	0.9800
C(51A)-H(51F)	0.9800
C(52A)-H(52D)	0.9800
C(52A)-H(52E)	0.9800
C(52A)-H(52F)	0.9800
C(53A)-H(53D)	0.9800
C(53A)-H(53E)	0.9800
C(53A)-H(53F)	0.9800

O(2)-Na(1)-N(3)	78.50(8)
O(2)-Na(1)-N(41)	106.52(10)

Electronic Supplementary Information

N(3)-Na(1)-N(41)	133.52(11)
O(2)-Na(1)-N(44)	122.03(9)
N(3)-Na(1)-N(44)	141.70(10)
N(41)-Na(1)-N(44)	75.45(9)
O(2)-Na(1)-C(42)	107.67(9)
N(3)-Na(1)-C(42)	160.30(10)
N(41)-Na(1)-C(42)	27.12(9)
N(44)-Na(1)-C(42)	50.97(9)
O(2)-Na(1)-Zn(1)	39.98(6)
N(3)-Na(1)-Zn(1)	38.55(6)
N(41)-Na(1)-Zn(1)	128.13(8)
N(44)-Na(1)-Zn(1)	149.47(8)
C(42)-Na(1)-Zn(1)	143.46(8)
N(3)-Zn(1)-C(1)	148.43(12)
N(3)-Zn(1)-O(2)	96.75(9)
C(1)-Zn(1)-O(2)	114.79(11)
N(3)-Zn(1)-Na(1)	51.26(8)
C(1)-Zn(1)-Na(1)	160.31(10)
O(2)-Zn(1)-Na(1)	45.53(6)
O(6)-Na(2)-N(7)	81.1(2)
O(6)-Na(2)-N(81)	110.58(10)
N(7)-Na(2)-N(81)	139.45(19)
O(6)-Na(2)-N(7A)	74.7(4)
N(7)-Na(2)-N(7A)	9.0(4)
N(81)-Na(2)-N(7A)	135.2(3)
O(6)-Na(2)-N(84)	120.50(10)
N(7)-Na(2)-N(84)	132.54(15)
N(81)-Na(2)-N(84)	76.21(11)
N(7A)-Na(2)-N(84)	141.4(3)
O(6)-Na(2)-Zn(2)	40.20(6)
N(7)-Na(2)-Zn(2)	40.88(19)
N(81)-Na(2)-Zn(2)	137.09(9)
N(7A)-Na(2)-Zn(2)	35.0(4)
N(84)-Na(2)-Zn(2)	140.77(8)
O(6)-Na(2)-C(83)	114.56(11)
N(7)-Na(2)-C(83)	158.80(17)
N(81)-Na(2)-C(83)	50.90(11)
N(7A)-Na(2)-C(83)	167.8(3)

Electronic Supplementary Information

N(84)-Na(2)-C(83)	27.53(10)
Zn(2)-Na(2)-C(83)	152.03(9)
N(7A)-Zn(2)-C(5A)	142.9(9)
N(7A)-Zn(2)-C(5)	145.6(9)
C(5A)-Zn(2)-C(5)	13.7(4)
N(7A)-Zn(2)-O(6)	98.2(9)
C(5A)-Zn(2)-O(6)	118.6(4)
C(5)-Zn(2)-O(6)	114.95(18)
N(7A)-Zn(2)-N(7)	9.6(6)
C(5A)-Zn(2)-N(7)	143.9(5)
C(5)-Zn(2)-N(7)	150.3(4)
O(6)-Zn(2)-N(7)	94.8(3)
N(7A)-Zn(2)-Na(2)	53.4(8)
C(5A)-Zn(2)-Na(2)	160.1(4)
C(5)-Zn(2)-Na(2)	160.44(18)
O(6)-Zn(2)-Na(2)	45.49(6)
N(7)-Zn(2)-Na(2)	49.3(3)
C(11)-C(1)-C(13)	109.0(3)
C(11)-C(1)-C(12)	108.6(3)
C(13)-C(1)-C(12)	108.2(3)
C(11)-C(1)-Zn(1)	110.0(2)
C(13)-C(1)-Zn(1)	111.0(2)
C(12)-C(1)-Zn(1)	110.0(2)
C(1)-C(11)-H(11A)	109.5
C(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(1)-C(12)-H(12A)	109.5
C(1)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(1)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(1)-C(13)-H(13A)	109.5
C(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5

C(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(21)-O(2)-Zn(1)	129.41(18)
C(21)-O(2)-Na(1)	136.10(19)
Zn(1)-O(2)-Na(1)	94.49(9)
O(2)-C(21)-C(22)	129.9(3)
O(2)-C(21)-C(213)	122.5(3)
C(22)-C(21)-C(213)	107.6(3)
C(21)-C(22)-C(23)	132.8(3)
C(21)-C(22)-C(27)	110.1(3)
C(23)-C(22)-C(27)	116.9(3)
C(24)-C(23)-C(22)	121.3(3)
C(24)-C(23)-H(63A)	119.4
C(22)-C(23)-H(63A)	119.4
C(23)-C(24)-C(25)	123.4(3)
C(23)-C(24)-H(64A)	118.3
C(25)-C(24)-H(64A)	118.3
C(26)-C(25)-C(24)	111.0(3)
C(26)-C(25)-C(20)	111.7(3)
C(24)-C(25)-C(20)	111.5(3)
C(26)-C(25)-H(25A)	107.5
C(24)-C(25)-H(25A)	107.5
C(20)-C(25)-H(25A)	107.5
C(27)-C(26)-C(25)	122.3(3)
C(27)-C(26)-H(66A)	118.9
C(25)-C(26)-H(66A)	118.9
C(26)-C(27)-C(22)	123.2(3)
C(26)-C(27)-C(28)	130.3(3)
C(22)-C(27)-C(28)	106.5(3)
C(29)-C(28)-C(213)	119.9(3)
C(29)-C(28)-C(27)	132.9(3)
C(213)-C(28)-C(27)	107.2(3)
C(28)-C(29)-C(210)	119.0(3)
C(28)-C(29)-H(69A)	120.5
C(210)-C(29)-H(69A)	120.5
C(211)-C(210)-C(29)	120.4(3)
C(211)-C(210)-H(61J)	119.8

C(29)-C(210)-H(61J)	119.8
C(212)-C(211)-C(210)	121.2(3)
C(212)-C(211)-H(61K)	119.4
C(210)-C(211)-H(61K)	119.4
C(213)-C(212)-C(211)	119.2(3)
C(213)-C(212)-H(61L)	120.4
C(211)-C(212)-H(61L)	120.4
C(212)-C(213)-C(28)	120.3(3)
C(212)-C(213)-C(21)	131.1(3)
C(28)-C(213)-C(21)	108.6(3)
C(215)-C(20)-C(216)	108.4(3)
C(215)-C(20)-C(25)	111.2(4)
C(216)-C(20)-C(25)	110.1(3)
C(215)-C(20)-C(214)	108.9(3)
C(216)-C(20)-C(214)	109.5(4)
C(25)-C(20)-C(214)	108.8(3)
C(20)-C(214)-H(61G)	109.5
C(20)-C(214)-H(61H)	109.5
H(61G)-C(214)-H(61H)	109.5
C(20)-C(214)-H(61I)	109.5
H(61G)-C(214)-H(61I)	109.5
H(61H)-C(214)-H(61I)	109.5
C(20)-C(215)-H(61D)	109.5
C(20)-C(215)-H(61E)	109.5
H(61D)-C(215)-H(61E)	109.5
C(20)-C(215)-H(61F)	109.5
H(61D)-C(215)-H(61F)	109.5
H(61E)-C(215)-H(61F)	109.5
C(20)-C(216)-H(61A)	109.5
C(20)-C(216)-H(61B)	109.5
H(61A)-C(216)-H(61B)	109.5
C(20)-C(216)-H(61C)	109.5
H(61A)-C(216)-H(61C)	109.5
H(61B)-C(216)-H(61C)	109.5
C(35)-N(3)-C(31)	116.8(3)
C(35)-N(3)-Zn(1)	112.81(18)
C(31)-N(3)-Zn(1)	113.54(19)
C(35)-N(3)-Na(1)	112.24(19)

C(31)-N(3)-Na(1)	108.03(18)
Zn(1)-N(3)-Na(1)	90.19(10)
N(3)-C(31)-C(311)	107.1(3)
N(3)-C(31)-C(32)	112.1(3)
C(311)-C(31)-C(32)	108.8(3)
N(3)-C(31)-C(312)	112.2(3)
C(311)-C(31)-C(312)	107.6(3)
C(32)-C(31)-C(312)	108.9(3)
C(31)-C(311)-H(71A)	109.5
C(31)-C(311)-H(71B)	109.5
H(71A)-C(311)-H(71B)	109.5
C(31)-C(311)-H(71C)	109.5
H(71A)-C(311)-H(71C)	109.5
H(71B)-C(311)-H(71C)	109.5
C(31)-C(312)-H(71D)	109.5
C(31)-C(312)-H(71E)	109.5
H(71D)-C(312)-H(71E)	109.5
C(31)-C(312)-H(71F)	109.5
H(71D)-C(312)-H(71F)	109.5
H(71E)-C(312)-H(71F)	109.5
C(33)-C(32)-C(31)	112.9(3)
C(33)-C(32)-H(72A)	109.0
C(31)-C(32)-H(72A)	109.0
C(33)-C(32)-H(72B)	109.0
C(31)-C(32)-H(72B)	109.0
H(72A)-C(32)-H(72B)	107.8
C(32)-C(33)-C(34)	109.4(3)
C(32)-C(33)-H(73A)	109.8
C(34)-C(33)-H(73A)	109.8
C(32)-C(33)-H(73B)	109.8
C(34)-C(33)-H(73B)	109.8
H(73A)-C(33)-H(73B)	108.2
C(33)-C(34)-C(35)	112.8(3)
C(33)-C(34)-H(74A)	109.0
C(35)-C(34)-H(74A)	109.0
C(33)-C(34)-H(74B)	109.0
C(35)-C(34)-H(74B)	109.0
H(74A)-C(34)-H(74B)	107.8

N(3)-C(35)-C(351)	107.3(3)
N(3)-C(35)-C(34)	112.6(3)
C(351)-C(35)-C(34)	107.7(3)
N(3)-C(35)-C(352)	113.1(2)
C(351)-C(35)-C(352)	106.2(3)
C(34)-C(35)-C(352)	109.5(3)
C(35)-C(351)-H(75A)	109.5
C(35)-C(351)-H(75B)	109.5
H(75A)-C(351)-H(75B)	109.5
C(35)-C(351)-H(75C)	109.5
H(75A)-C(351)-H(75C)	109.5
H(75B)-C(351)-H(75C)	109.5
C(35)-C(352)-H(75D)	109.5
C(35)-C(352)-H(75E)	109.5
H(75D)-C(352)-H(75E)	109.5
C(35)-C(352)-H(75F)	109.5
H(75D)-C(352)-H(75F)	109.5
H(75E)-C(352)-H(75F)	109.5
C(411)-N(41)-C(42)	110.0(3)
C(411)-N(41)-C(412)	109.4(3)
C(42)-N(41)-C(412)	109.7(3)
C(411)-N(41)-Na(1)	117.6(2)
C(42)-N(41)-Na(1)	103.0(2)
C(412)-N(41)-Na(1)	106.8(2)
N(41)-C(411)-H(81A)	109.5
N(41)-C(411)-H(81B)	109.5
H(81A)-C(411)-H(81B)	109.5
N(41)-C(411)-H(81C)	109.5
H(81A)-C(411)-H(81C)	109.5
H(81B)-C(411)-H(81C)	109.5
N(41)-C(412)-H(81D)	109.5
N(41)-C(412)-H(81E)	109.5
H(81D)-C(412)-H(81E)	109.5
N(41)-C(412)-H(81F)	109.5
H(81D)-C(412)-H(81F)	109.5
H(81E)-C(412)-H(81F)	109.5
N(41)-C(42)-C(43)	114.2(3)
N(41)-C(42)-Na(1)	49.90(16)

Electronic Supplementary Information

C(43)-C(42)-Na(1)	80.00(19)
N(41)-C(42)-H(82A)	108.7
C(43)-C(42)-H(82A)	108.7
Na(1)-C(42)-H(82A)	157.7
N(41)-C(42)-H(82B)	108.7
C(43)-C(42)-H(82B)	108.7
Na(1)-C(42)-H(82B)	87.9
H(82A)-C(42)-H(82B)	107.6
N(44)-C(43)-C(42)	114.9(3)
N(44)-C(43)-H(83A)	108.5
C(42)-C(43)-H(83A)	108.5
N(44)-C(43)-H(83B)	108.5
C(42)-C(43)-H(83B)	108.5
H(83A)-C(43)-H(83B)	107.5
C(442)-N(44)-C(43)	109.2(2)
C(442)-N(44)-C(441)	108.7(3)
C(43)-N(44)-C(441)	110.2(3)
C(442)-N(44)-Na(1)	120.6(2)
C(43)-N(44)-Na(1)	105.13(19)
C(441)-N(44)-Na(1)	102.56(19)
N(44)-C(441)-H(84A)	109.5
N(44)-C(441)-H(84B)	109.5
H(84A)-C(441)-H(84B)	109.5
N(44)-C(441)-H(84C)	109.5
H(84A)-C(441)-H(84C)	109.5
H(84B)-C(441)-H(84C)	109.5
N(44)-C(442)-H(84D)	109.5
N(44)-C(442)-H(84E)	109.5
H(84D)-C(442)-H(84E)	109.5
N(44)-C(442)-H(84F)	109.5
H(84D)-C(442)-H(84F)	109.5
H(84E)-C(442)-H(84F)	109.5
C(51)-C(5)-C(53)	108.6(5)
C(51)-C(5)-C(52)	109.2(8)
C(53)-C(5)-C(52)	110.3(9)
C(51)-C(5)-Zn(2)	108.9(4)
C(53)-C(5)-Zn(2)	112.1(4)
C(52)-C(5)-Zn(2)	107.7(6)

Electronic Supplementary Information

C(61)-O(6)-Zn(2)	128.63(19)
C(61)-O(6)-Na(2)	137.1(2)
Zn(2)-O(6)-Na(2)	94.31(9)
O(6)-C(61)-C(62)	128.9(3)
O(6)-C(61)-C(613)	122.8(3)
C(62)-C(61)-C(613)	108.3(3)
C(61)-C(62)-C(63)	133.7(4)
C(61)-C(62)-C(67)	108.9(3)
C(63)-C(62)-C(67)	117.3(3)
C(64)-C(63)-C(62)	121.2(4)
C(64)-C(63)-H(23A)	119.4
C(62)-C(63)-H(23A)	119.4
C(63)-C(64)-C(65)	124.9(4)
C(63)-C(64)-H(24A)	117.6
C(65)-C(64)-H(24A)	117.6
C(66)-C(65)-C(64)	111.1(3)
C(66)-C(65)-C(60)	111.6(3)
C(64)-C(65)-C(60)	113.2(3)
C(66)-C(65)-H(65A)	106.8
C(64)-C(65)-H(65A)	106.8
C(60)-C(65)-H(65A)	106.8
C(67)-C(66)-C(65)	122.5(3)
C(67)-C(66)-H(26A)	118.7
C(65)-C(66)-H(26A)	118.7
C(66)-C(67)-C(62)	122.6(4)
C(66)-C(67)-C(68)	130.5(3)
C(62)-C(67)-C(68)	106.9(3)
C(69)-C(68)-C(613)	120.8(3)
C(69)-C(68)-C(67)	132.4(3)
C(613)-C(68)-C(67)	106.8(3)
C(610)-C(69)-C(68)	118.4(3)
C(610)-C(69)-H(29A)	120.8
C(68)-C(69)-H(29A)	120.8
C(611)-C(610)-C(69)	120.5(3)
C(611)-C(610)-H(21J)	119.8
C(69)-C(610)-H(21J)	119.8
C(610)-C(611)-C(612)	121.3(4)
C(610)-C(611)-H(21K)	119.4

C(612)-C(611)-H(21K)	119.4
C(613)-C(612)-C(611)	118.8(3)
C(613)-C(612)-H(21L)	120.6
C(611)-C(612)-H(21L)	120.6
C(612)-C(613)-C(68)	120.2(3)
C(612)-C(613)-C(61)	130.7(3)
C(68)-C(613)-C(61)	109.1(3)
C(616)-C(60)-C(615)	108.1(3)
C(616)-C(60)-C(65)	111.6(3)
C(615)-C(60)-C(65)	110.4(3)
C(616)-C(60)-C(614)	108.4(3)
C(615)-C(60)-C(614)	109.6(3)
C(65)-C(60)-C(614)	108.6(3)
C(60)-C(614)-H(21A)	109.5
C(60)-C(614)-H(21B)	109.5
H(21A)-C(614)-H(21B)	109.5
C(60)-C(614)-H(21C)	109.5
H(21A)-C(614)-H(21C)	109.5
H(21B)-C(614)-H(21C)	109.5
C(60)-C(615)-H(21D)	109.5
C(60)-C(615)-H(21E)	109.5
H(21D)-C(615)-H(21E)	109.5
C(60)-C(615)-H(21F)	109.5
H(21D)-C(615)-H(21F)	109.5
H(21E)-C(615)-H(21F)	109.5
C(60)-C(616)-H(21G)	109.5
C(60)-C(616)-H(21H)	109.5
H(21G)-C(616)-H(21H)	109.5
C(60)-C(616)-H(21I)	109.5
H(21G)-C(616)-H(21I)	109.5
H(21H)-C(616)-H(21I)	109.5
C(71)-N(7)-C(75)	116.5(6)
C(71)-N(7)-Zn(2)	107.9(4)
C(75)-N(7)-Zn(2)	113.9(5)
C(71)-N(7)-Na(2)	118.7(6)
C(75)-N(7)-Na(2)	107.2(5)
Zn(2)-N(7)-Na(2)	89.8(3)
N(7)-C(71)-C(72)	114.1(6)

N(7)-C(71)-C(711)	108.3(4)
C(72)-C(71)-C(711)	108.0(4)
N(7)-C(71)-C(712)	111.8(8)
C(72)-C(71)-C(712)	112.4(6)
C(711)-C(71)-C(712)	101.4(5)
C(73)-C(72)-C(71)	111.7(4)
C(73)-C(72)-H(32A)	109.3
C(71)-C(72)-H(32A)	109.3
C(73)-C(72)-H(32B)	109.3
C(71)-C(72)-H(32B)	109.3
H(32A)-C(72)-H(32B)	107.9
C(72)-C(73)-C(74)	112.4(5)
C(72)-C(73)-H(33A)	109.1
C(74)-C(73)-H(33A)	109.1
C(72)-C(73)-H(33B)	109.1
C(74)-C(73)-H(33B)	109.1
H(33A)-C(73)-H(33B)	107.9
C(75)-C(74)-C(73)	112.3(5)
C(75)-C(74)-H(34A)	109.1
C(73)-C(74)-H(34A)	109.1
C(75)-C(74)-H(34B)	109.1
C(73)-C(74)-H(34B)	109.1
H(34A)-C(74)-H(34B)	107.9
N(7)-C(75)-C(752)	108.4(5)
N(7)-C(75)-C(751)	111.6(5)
C(752)-C(75)-C(751)	103.7(5)
N(7)-C(75)-C(74)	112.6(6)
C(752)-C(75)-C(74)	110.2(5)
C(751)-C(75)-C(74)	109.9(5)
C(100)-N(7A)-C(104)	116.6(12)
C(100)-N(7A)-Zn(2)	122.6(10)
C(104)-N(7A)-Zn(2)	111.0(11)
C(100)-N(7A)-Na(2)	106.2(13)
C(104)-N(7A)-Na(2)	103.2(11)
Zn(2)-N(7A)-Na(2)	91.7(8)
N(7A)-C(100)-C(106)	105.8(10)
N(7A)-C(100)-C(105)	111.7(13)
C(106)-C(100)-C(105)	109.3(9)

N(7A)-C(100)-C(101)	112.5(13)
C(106)-C(100)-C(101)	113.7(10)
C(105)-C(100)-C(101)	104.0(12)
C(102)-C(101)-C(100)	111.5(10)
C(102)-C(101)-H(10A)	109.3
C(100)-C(101)-H(10A)	109.3
C(102)-C(101)-H(10B)	109.3
C(100)-C(101)-H(10B)	109.3
H(10A)-C(101)-H(10B)	108.0
C(101)-C(102)-C(103)	117.4(13)
C(101)-C(102)-H(10C)	107.9
C(103)-C(102)-H(10C)	107.9
C(101)-C(102)-H(10D)	107.9
C(103)-C(102)-H(10D)	107.9
H(10C)-C(102)-H(10D)	107.2
C(102)-C(103)-C(104)	105.9(9)
C(102)-C(103)-H(10E)	110.5
C(104)-C(103)-H(10E)	110.5
C(102)-C(103)-H(10F)	110.5
C(104)-C(103)-H(10F)	110.5
H(10E)-C(103)-H(10F)	108.7
N(7A)-C(104)-C(103)	113.2(12)
N(7A)-C(104)-C(107)	106.1(10)
C(103)-C(104)-C(107)	116.9(10)
N(7A)-C(104)-C(108)	111.6(13)
C(103)-C(104)-C(108)	105.4(9)
C(107)-C(104)-C(108)	103.4(8)
C(100)-C(105)-H(10G)	109.5
C(100)-C(105)-H(10H)	109.5
H(10G)-C(105)-H(10H)	109.5
C(100)-C(105)-H(10I)	109.5
H(10G)-C(105)-H(10I)	109.5
H(10H)-C(105)-H(10I)	109.5
C(100)-C(106)-H(10J)	109.5
C(100)-C(106)-H(10K)	109.5
H(10J)-C(106)-H(10K)	109.5
C(100)-C(106)-H(10L)	109.5
H(10J)-C(106)-H(10L)	109.5

H(10K)-C(106)-H(10L)	109.5
C(104)-C(107)-H(10M)	109.5
C(104)-C(107)-H(10N)	109.5
H(10M)-C(107)-H(10N)	109.5
C(104)-C(107)-H(10O)	109.5
H(10M)-C(107)-H(10O)	109.5
H(10N)-C(107)-H(10O)	109.5
C(104)-C(108)-H(10P)	109.5
C(104)-C(108)-H(10Q)	109.5
H(10P)-C(108)-H(10Q)	109.5
C(104)-C(108)-H(10R)	109.5
H(10P)-C(108)-H(10R)	109.5
H(10Q)-C(108)-H(10R)	109.5
C(812)-N(81)-C(811)	108.4(3)
C(812)-N(81)-C(82)	109.2(3)
C(811)-N(81)-C(82)	111.2(2)
C(812)-N(81)-Na(2)	119.8(2)
C(811)-N(81)-Na(2)	101.79(8)
C(82)-N(81)-Na(2)	106.2(2)
N(81)-C(811)-H(41A)	109.5
N(81)-C(811)-H(41B)	109.5
H(41A)-C(811)-H(41B)	109.5
N(81)-C(811)-H(41C)	109.5
H(41A)-C(811)-H(41C)	109.5
H(41B)-C(811)-H(41C)	109.4
N(81)-C(812)-H(41D)	109.5
N(81)-C(812)-H(41E)	109.5
H(41D)-C(812)-H(41E)	109.5
N(81)-C(812)-H(41F)	109.5
H(41D)-C(812)-H(41F)	109.5
H(41E)-C(812)-H(41F)	109.5
C(83)-C(82)-N(81)	116.4(3)
C(83)-C(82)-H(42A)	108.2
N(81)-C(82)-H(42A)	108.2
C(83)-C(82)-H(42B)	108.2
N(81)-C(82)-H(42B)	108.2
H(42A)-C(82)-H(42B)	107.3
C(82)-C(83)-N(84)	116.3(4)

C(82)-C(83)-Na(2)	78.5(2)
N(84)-C(83)-Na(2)	52.13(18)
C(82)-C(83)-H(43A)	108.2
N(84)-C(83)-H(43A)	108.2
Na(2)-C(83)-H(43A)	158.5
C(82)-C(83)-H(43B)	108.2
N(84)-C(83)-H(43B)	108.2
Na(2)-C(83)-H(43B)	89.0
H(43A)-C(83)-H(43B)	107.4
C(841)-N(84)-C(842)	108.8(3)
C(841)-N(84)-C(83)	111.4(3)
C(842)-N(84)-C(83)	106.9(3)
C(841)-N(84)-Na(2)	117.4(2)
C(842)-N(84)-Na(2)	111.3(2)
C(83)-N(84)-Na(2)	100.3(2)
N(84)-C(841)-H(44A)	109.5
N(84)-C(841)-H(44B)	109.5
H(44A)-C(841)-H(44B)	109.5
N(84)-C(841)-H(44C)	109.5
H(44A)-C(841)-H(44C)	109.5
H(44B)-C(841)-H(44C)	109.5
N(84)-C(842)-H(44D)	109.5
N(84)-C(842)-H(44E)	109.5
H(44D)-C(842)-H(44E)	109.5
N(84)-C(842)-H(44F)	109.5
H(44D)-C(842)-H(44F)	109.5
H(44E)-C(842)-H(44F)	109.5
C(52A)-C(5A)-C(53A)	110.1(19)
C(52A)-C(5A)-C(51A)	111.1(11)
C(53A)-C(5A)-C(51A)	99.2(17)
C(52A)-C(5A)-Zn(2)	115.1(10)
C(53A)-C(5A)-Zn(2)	119.5(17)
C(51A)-C(5A)-Zn(2)	99.7(9)
C(5A)-C(51A)-H(51D)	109.5
C(5A)-C(51A)-H(51E)	109.5
H(51D)-C(51A)-H(51E)	109.5
C(5A)-C(51A)-H(51F)	109.5
H(51D)-C(51A)-H(51F)	109.5

H(51E)-C(51A)-H(51F)	109.5
C(5A)-C(52A)-H(52D)	109.5
C(5A)-C(52A)-H(52E)	109.5
H(52D)-C(52A)-H(52E)	109.5
C(5A)-C(52A)-H(52F)	109.5
H(52D)-C(52A)-H(52F)	109.5
H(52E)-C(52A)-H(52F)	109.5
C(5A)-C(53A)-H(53D)	109.5
C(5A)-C(53A)-H(53E)	109.5
H(53D)-C(53A)-H(53E)	109.5
C(5A)-C(53A)-H(53F)	109.5
H(53D)-C(53A)-H(53F)	109.5
H(53E)-C(53A)-H(53F)	109.5

Symmetry transformations used to generate equivalent atoms:

Electronic Supplementary Information

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for jksamboth. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Na(1)	29(1)	30(1)	34(1)	-6(1)	3(1)	8(1)
Zn(1)	21(1)	25(1)	35(1)	1(1)	4(1)	1(1)
Na(2)	30(1)	29(1)	40(1)	-1(1)	2(1)	1(1)
Zn(2)	25(1)	35(1)	62(1)	-12(1)	-8(1)	2(1)
C(1)	26(2)	27(2)	39(3)	-1(2)	3(2)	3(2)
C(11)	27(2)	47(3)	106(4)	3(3)	32(2)	4(2)
C(12)	28(2)	53(3)	60(3)	-5(2)	-2(2)	12(2)
C(13)	34(2)	42(3)	59(3)	-9(2)	10(2)	5(2)
O(2)	28(1)	25(1)	41(2)	-8(1)	8(1)	-8(1)
C(21)	27(2)	26(2)	30(2)	-5(2)	8(2)	-2(2)
C(22)	41(2)	23(2)	33(2)	7(2)	6(2)	-7(2)
C(23)	50(2)	34(2)	48(3)	3(2)	3(2)	-12(2)
C(24)	49(2)	48(3)	48(3)	17(2)	6(2)	-2(2)
C(25)	37(2)	51(3)	52(3)	9(3)	2(2)	-7(2)
C(26)	37(2)	39(3)	45(3)	6(2)	5(2)	-6(2)
C(27)	31(2)	29(2)	31(3)	0(2)	4(2)	-4(2)
C(28)	24(2)	22(2)	29(2)	2(2)	9(2)	4(2)
C(29)	25(2)	30(2)	33(3)	-2(2)	10(2)	2(2)
C(210)	34(2)	33(2)	45(3)	8(2)	13(2)	0(2)
C(211)	36(2)	52(3)	25(2)	9(2)	4(2)	7(2)
C(212)	24(2)	36(2)	38(3)	0(2)	9(2)	2(2)
C(213)	23(2)	27(2)	25(2)	-2(2)	9(2)	6(2)
C(20)	66(3)	49(3)	39(3)	0(2)	10(2)	-9(2)
C(214)	66(3)	99(4)	82(4)	-6(3)	19(3)	4(3)
C(215)	102(3)	87(4)	36(3)	13(3)	-7(2)	-40(3)
C(216)	116(4)	72(4)	37(3)	-9(3)	16(2)	-25(3)
N(3)	23(1)	26(2)	29(2)	0(2)	7(1)	1(1)
C(31)	21(2)	28(2)	36(3)	3(2)	9(2)	-2(2)
C(311)	27(2)	44(3)	47(3)	18(2)	6(2)	3(2)
C(312)	35(2)	37(2)	44(3)	-1(2)	10(2)	-5(2)
C(32)	43(2)	27(2)	69(3)	3(2)	21(2)	1(2)
C(33)	66(3)	33(3)	77(4)	-24(3)	28(3)	-7(2)
C(34)	50(2)	53(3)	45(3)	-18(2)	14(2)	-5(2)

Electronic Supplementary Information

C(35)	29(2)	32(2)	29(2)	-10(2)	6(2)	-4(2)
C(351)	45(2)	52(3)	34(3)	9(2)	4(2)	-1(2)
C(352)	38(2)	63(3)	38(3)	3(2)	-4(2)	6(2)
N(41)	47(2)	32(2)	35(2)	3(2)	4(2)	14(2)
C(411)	93(3)	56(3)	72(3)	-2(3)	50(3)	1(3)
C(412)	80(3)	83(4)	49(3)	-8(3)	-7(2)	40(3)
C(42)	57(2)	40(3)	31(3)	-7(2)	10(2)	10(2)
C(43)	45(2)	43(3)	44(3)	3(2)	10(2)	20(2)
N(44)	26(2)	32(2)	28(2)	-4(2)	6(1)	1(1)
C(441)	60(3)	46(3)	45(3)	-4(2)	8(2)	-12(2)
C(442)	37(2)	44(3)	43(3)	2(2)	1(2)	6(2)
C(51)	19(3)	76(5)	78(5)	-40(4)	-17(3)	11(3)
C(52)	43(5)	46(4)	97(9)	-30(4)	-7(6)	28(3)
C(53)	26(3)	84(5)	66(4)	-20(4)	7(3)	13(3)
O(6)	29(1)	29(2)	59(2)	-3(1)	4(1)	-8(1)
C(61)	25(2)	25(2)	44(3)	-2(2)	1(2)	3(2)
C(62)	34(2)	33(2)	34(3)	-4(2)	-6(2)	-5(2)
C(63)	64(3)	47(3)	46(3)	2(3)	-10(2)	-17(2)
C(64)	81(3)	51(3)	36(3)	-2(2)	-9(2)	-8(3)
C(65)	57(3)	46(3)	37(3)	2(2)	2(2)	3(2)
C(66)	49(2)	39(3)	42(3)	-2(2)	0(2)	-12(2)
C(67)	38(2)	29(2)	37(3)	0(2)	1(2)	-8(2)
C(68)	24(2)	23(2)	33(3)	-5(2)	1(2)	2(2)
C(69)	26(2)	30(2)	38(3)	-1(2)	2(2)	-2(2)
C(610)	37(2)	38(3)	28(3)	-4(2)	-3(2)	6(2)
C(611)	40(2)	40(3)	35(3)	8(2)	10(2)	13(2)
C(612)	28(2)	29(2)	43(3)	0(2)	7(2)	-2(2)
C(613)	22(2)	26(2)	33(3)	-2(2)	7(2)	3(2)
C(60)	52(3)	49(3)	32(3)	4(2)	5(2)	0(2)
C(614)	59(3)	88(4)	51(3)	-6(3)	10(2)	8(3)
C(615)	89(3)	61(3)	38(3)	6(2)	13(2)	6(3)
C(616)	62(3)	40(3)	59(3)	1(2)	19(2)	-6(2)
N(7)	19(4)	33(2)	18(3)	-1(3)	8(3)	-1(2)
N(7A)	19(4)	33(2)	18(3)	-1(3)	8(3)	-1(2)
N(81)	48(2)	50(2)	42(2)	8(2)	4(2)	14(2)
C(811)	90(3)	59(3)	100(4)	32(3)	22(3)	12(3)
C(812)	96(4)	117(5)	75(4)	-11(3)	-36(3)	52(3)
C(82)	79(3)	46(3)	80(4)	-9(3)	8(3)	23(3)

Electronic Supplementary Information

C(83)	75(3)	74(4)	68(4)	-24(3)	1(3)	22(3)
N(84)	36(2)	52(2)	38(2)	-5(2)	5(2)	3(2)
C(841)	56(3)	111(4)	91(4)	-19(3)	32(3)	-34(3)
C(842)	52(3)	107(4)	54(3)	-22(3)	-3(2)	7(3)

Electronic Supplementary Information

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for jksamboth.

	x	y	z	U(eq)
H(11A)	-2292	5434	1983	88
H(11B)	-1007	5140	2207	88
H(11C)	-1328	4938	1788	88
H(12A)	-2096	6297	1499	71
H(12B)	-1157	5786	1304	71
H(12C)	-678	6544	1402	71
H(13A)	-1652	6610	2134	67
H(13B)	-231	6884	2057	67
H(13C)	-380	6336	2371	67
H(63A)	290	5153	849	53
H(64A)	-1079	4924	347	58
H(25A)	-2544	3983	378	56
H(66A)	-2116	3092	815	49
H(69A)	-1705	2440	1451	35
H(61J)	-1091	2129	2054	44
H(61K)	363	2795	2416	45
H(61L)	1254	3776	2186	39
H(61G)	866	3126	76	123
H(61H)	641	3220	497	123
H(61I)	907	3870	253	123
H(61D)	-2155	3891	-283	113
H(61E)	-764	3628	-393	113
H(61F)	-866	4334	-181	113
H(61A)	-2585	2838	77	112
H(61B)	-1387	2518	328	112
H(61C)	-1320	2565	-104	112
H(71A)	2848	5997	1240	59
H(71B)	3071	6798	1196	59
H(71C)	1841	6525	1394	59
H(71D)	5166	5930	1533	57
H(71E)	5592	6420	1869	57
H(71F)	5261	6734	1471	57

Electronic Supplementary Information

H(72A)	3826	7501	1763	54
H(72B)	2451	7250	1890	54
H(73A)	3778	7609	2402	69
H(73B)	4921	7099	2306	69
H(74A)	2397	6693	2511	58
H(74B)	3747	6598	2758	58
H(75A)	1712	5562	2483	66
H(75B)	2887	5377	2781	66
H(75C)	2684	4949	2411	66
H(75D)	5057	5205	2315	70
H(75E)	5078	5581	2700	70
H(75F)	5552	5975	2355	70
H(81A)	5850	4715	715	107
H(81B)	6323	4888	1130	107
H(81C)	5331	5387	901	107
H(81D)	3555	4432	556	108
H(81E)	3127	5099	765	108
H(81F)	2595	4368	875	108
H(82A)	5251	3666	879	51
H(82B)	4014	3546	1108	51
H(83A)	5956	3162	1419	52
H(83B)	6541	3915	1416	52
H(84A)	4674	2816	1856	76
H(84B)	3502	3270	1670	76
H(84C)	3936	3347	2096	76
H(84D)	6697	3357	2071	62
H(84E)	5895	3884	2297	62
H(84F)	6876	4158	2015	62
H(51A)	7959	4490	6130	88
H(51B)	6905	4390	6422	88
H(51C)	6908	5074	6187	88
H(52A)	5639	3266	5730	94
H(52B)	6093	3319	6156	94
H(52C)	7159	3351	5863	94
H(53A)	6388	5016	5517	88
H(53B)	5826	4328	5332	88
H(53C)	7339	4379	5478	88
H(23A)	4392	6070	5378	64

Electronic Supplementary Information

H(24A)	5369	6815	5034	68
H(65A)	7318	7334	5327	56
H(26A)	7398	7633	5965	52
H(29A)	7566	7448	6682	37
H(21J)	7429	7026	7272	42
H(21K)	6154	6079	7368	46
H(21L)	4919	5556	6885	40
H(21A)	4090	7896	5461	99
H(21B)	4339	8696	5425	99
H(21C)	4926	8296	5780	99
H(21D)	6486	8030	4799	93
H(21E)	5485	8640	4850	93
H(21F)	4972	7871	4838	93
H(21G)	7836	8547	5355	79
H(21H)	7112	8673	5717	79
H(21I)	6695	9103	5357	79
H(31A)	2197	4846	5400	58
H(31B)	2118	4199	5135	58
H(31C)	3407	4330	5403	58
H(31D)	-145	3690	5649	81
H(31E)	180	4218	5339	81
H(31F)	121	4473	5749	81
H(32A)	1695	3028	5383	44
H(32B)	3132	3140	5581	44
H(33A)	2138	2284	5871	50
H(33B)	882	2749	5920	50
H(34A)	2159	2728	6484	61
H(34B)	3446	2946	6295	61
H(35A)	790	3638	6722	68
H(35B)	196	3579	6307	68
H(35C)	569	4309	6479	68
H(35D)	3971	3981	6627	79
H(35E)	2902	3752	6895	79
H(35F)	2843	4499	6721	79
H(10A)	-57	4451	5667	40
H(10B)	-43	3833	5385	40
H(10C)	401	3062	5839	40
H(10D)	-814	3506	5945	40

Electronic Supplementary Information

H(10E)	703	3283	6468	88
H(10F)	531	4088	6401	88
H(10G)	2177	3094	5545	123
H(10H)	3210	3538	5345	123
H(10I)	1751	3440	5160	123
H(10J)	2118	5161	5518	103
H(10K)	1489	4795	5156	103
H(10L)	3019	4710	5277	103
H(10M)	4174	3920	6506	79
H(10N)	3202	3565	6767	79
H(10O)	3036	4355	6667	79
H(10P)	2465	2889	5888	116
H(10Q)	2377	2661	6302	116
H(10R)	3720	2958	6175	116
H(41A)	1235	7198	5782	124
H(41B)	2025	6566	5636	124
H(41C)	2279	6801	6051	124
H(41D)	-726	6640	5556	148
H(41E)	-1039	5889	5692	148
H(41F)	107	6007	5430	148
H(42A)	-274	7057	6195	82
H(42B)	-954	6337	6246	82
H(43A)	32	6737	6780	87
H(43B)	1409	6765	6608	87
H(44A)	-640	5763	7044	127
H(44B)	-49	5037	6949	127
H(44C)	-942	5446	6645	127
H(44D)	1471	6139	7243	107
H(44E)	2620	6111	6975	107
H(44F)	2086	5423	7141	107
H(51D)	6963	5042	5852	123
H(51E)	5903	4758	5544	123
H(51F)	7307	4401	5610	123
H(52D)	6575	3852	6535	121
H(52E)	6703	4656	6479	121
H(52F)	7787	4155	6340	121
H(53D)	7285	3368	5867	116
H(53E)	6085	3496	5567	116

Electronic Supplementary Information

H(53F)	5846	3111	5938	116

Table 6. Torsion angles [°] for jksamboth.

N(3)-Zn(1)-C(1)-C(11)	-135.4(3)
O(2)-Zn(1)-C(1)-C(11)	41.7(3)
N(3)-Zn(1)-C(1)-C(13)	-14.8(4)
O(2)-Zn(1)-C(1)-C(13)	162.4(2)
N(3)-Zn(1)-C(1)-C(12)	104.9(3)
O(2)-Zn(1)-C(1)-C(12)	-77.9(2)
N(3)-Zn(1)-O(2)-C(21)	178.1(3)
C(1)-Zn(1)-O(2)-C(21)	-0.4(3)
N(3)-Zn(1)-O(2)-Na(1)	-2.26(11)
C(1)-Zn(1)-O(2)-Na(1)	179.26(12)
N(3)-Na(1)-O(2)-C(21)	-178.6(3)
N(41)-Na(1)-O(2)-C(21)	49.1(3)
N(44)-Na(1)-O(2)-C(21)	-33.8(3)
C(42)-Na(1)-O(2)-C(21)	20.8(3)
N(3)-Na(1)-O(2)-Zn(1)	1.83(9)
N(41)-Na(1)-O(2)-Zn(1)	-130.45(10)
N(44)-Na(1)-O(2)-Zn(1)	146.65(10)
C(42)-Na(1)-O(2)-Zn(1)	-158.83(9)
Zn(1)-O(2)-C(21)-C(22)	82.5(4)
Na(1)-O(2)-C(21)-C(22)	-97.0(4)
Zn(1)-O(2)-C(21)-C(213)	-97.7(3)
Na(1)-O(2)-C(21)-C(213)	82.8(4)
O(2)-C(21)-C(22)-C(23)	-8.7(6)
C(213)-C(21)-C(22)-C(23)	171.5(3)
O(2)-C(21)-C(22)-C(27)	177.2(3)
C(213)-C(21)-C(22)-C(27)	-2.6(4)
C(21)-C(22)-C(23)-C(24)	-178.9(3)
C(27)-C(22)-C(23)-C(24)	-5.1(5)
C(22)-C(23)-C(24)-C(25)	-6.0(6)
C(23)-C(24)-C(25)-C(26)	14.8(5)
C(23)-C(24)-C(25)-C(20)	-110.5(4)
C(24)-C(25)-C(26)-C(27)	-13.7(5)
C(20)-C(25)-C(26)-C(27)	111.4(4)
C(25)-C(26)-C(27)-C(22)	4.1(5)
C(25)-C(26)-C(27)-C(28)	-177.1(3)
C(21)-C(22)-C(27)-C(26)	-178.8(3)

Electronic Supplementary Information

C(23)-C(22)-C(27)-C(26)	6.1(5)
C(21)-C(22)-C(27)-C(28)	2.2(4)
C(23)-C(22)-C(27)-C(28)	-172.9(3)
C(26)-C(27)-C(28)-C(29)	-0.2(6)
C(22)-C(27)-C(28)-C(29)	178.7(3)
C(26)-C(27)-C(28)-C(213)	-179.8(3)
C(22)-C(27)-C(28)-C(213)	-0.9(3)
C(213)-C(28)-C(29)-C(210)	1.6(4)
C(27)-C(28)-C(29)-C(210)	-178.0(3)
C(28)-C(29)-C(210)-C(211)	-0.5(5)
C(29)-C(210)-C(211)-C(212)	-0.5(5)
C(210)-C(211)-C(212)-C(213)	0.3(5)
C(211)-C(212)-C(213)-C(28)	0.9(5)
C(211)-C(212)-C(213)-C(21)	179.0(3)
C(29)-C(28)-C(213)-C(212)	-1.8(4)
C(27)-C(28)-C(213)-C(212)	177.9(3)
C(29)-C(28)-C(213)-C(21)	179.7(3)
C(27)-C(28)-C(213)-C(21)	-0.7(3)
O(2)-C(21)-C(213)-C(212)	3.9(5)
C(22)-C(21)-C(213)-C(212)	-176.3(3)
O(2)-C(21)-C(213)-C(28)	-177.8(3)
C(22)-C(21)-C(213)-C(28)	2.0(3)
C(26)-C(25)-C(20)-C(215)	171.6(3)
C(24)-C(25)-C(20)-C(215)	-63.5(4)
C(26)-C(25)-C(20)-C(216)	51.5(4)
C(24)-C(25)-C(20)-C(216)	176.4(3)
C(26)-C(25)-C(20)-C(214)	-68.5(4)
C(24)-C(25)-C(20)-C(214)	56.3(4)
C(1)-Zn(1)-N(3)-C(35)	65.1(3)
O(2)-Zn(1)-N(3)-C(35)	-112.3(2)
C(1)-Zn(1)-N(3)-C(31)	-70.7(3)
O(2)-Zn(1)-N(3)-C(31)	111.9(2)
C(1)-Zn(1)-N(3)-Na(1)	179.4(2)
O(2)-Zn(1)-N(3)-Na(1)	2.06(10)
O(2)-Na(1)-N(3)-C(35)	112.96(19)
N(41)-Na(1)-N(3)-C(35)	-145.09(19)
N(44)-Na(1)-N(3)-C(35)	-15.0(3)
C(42)-Na(1)-N(3)-C(35)	-136.5(3)

Electronic Supplementary Information

O(2)-Na(1)-N(3)-C(31)	-116.79(19)
N(41)-Na(1)-N(3)-C(31)	-14.8(2)
N(44)-Na(1)-N(3)-C(31)	115.2(2)
C(42)-Na(1)-N(3)-C(31)	-6.3(4)
O(2)-Na(1)-N(3)-Zn(1)	-1.88(9)
N(41)-Na(1)-N(3)-Zn(1)	100.06(13)
N(44)-Na(1)-N(3)-Zn(1)	-129.88(14)
C(42)-Na(1)-N(3)-Zn(1)	108.6(3)
C(35)-N(3)-C(31)-C(311)	-164.0(2)
Zn(1)-N(3)-C(31)-C(311)	-30.0(3)
Na(1)-N(3)-C(31)-C(311)	68.4(2)
C(35)-N(3)-C(31)-C(32)	-44.8(3)
Zn(1)-N(3)-C(31)-C(32)	89.2(3)
Na(1)-N(3)-C(31)-C(32)	-172.4(2)
C(35)-N(3)-C(31)-C(312)	78.2(3)
Zn(1)-N(3)-C(31)-C(312)	-147.8(2)
Na(1)-N(3)-C(31)-C(312)	-49.5(3)
N(3)-C(31)-C(32)-C(33)	50.8(4)
C(311)-C(31)-C(32)-C(33)	169.1(3)
C(312)-C(31)-C(32)-C(33)	-74.0(4)
C(31)-C(32)-C(33)-C(34)	-56.6(4)
C(32)-C(33)-C(34)-C(35)	56.0(4)
C(31)-N(3)-C(35)-C(351)	162.8(3)
Zn(1)-N(3)-C(35)-C(351)	28.5(3)
Na(1)-N(3)-C(35)-C(351)	-71.6(3)
C(31)-N(3)-C(35)-C(34)	44.5(3)
Zn(1)-N(3)-C(35)-C(34)	-89.8(3)
Na(1)-N(3)-C(35)-C(34)	170.0(2)
C(31)-N(3)-C(35)-C(352)	-80.4(3)
Zn(1)-N(3)-C(35)-C(352)	145.3(2)
Na(1)-N(3)-C(35)-C(352)	45.2(3)
C(33)-C(34)-C(35)-N(3)	-49.9(4)
C(33)-C(34)-C(35)-C(351)	-167.9(3)
C(33)-C(34)-C(35)-C(352)	76.9(4)
O(2)-Na(1)-N(41)-C(411)	142.3(2)
N(3)-Na(1)-N(41)-C(411)	52.6(3)
N(44)-Na(1)-N(41)-C(411)	-98.1(3)
C(42)-Na(1)-N(41)-C(411)	-121.1(3)

Electronic Supplementary Information

O(2)-Na(1)-N(41)-C(42)	-96.6(2)
N(3)-Na(1)-N(41)-C(42)	173.67(18)
N(44)-Na(1)-N(41)-C(42)	23.02(19)
O(2)-Na(1)-N(41)-C(412)	18.9(3)
N(3)-Na(1)-N(41)-C(412)	-70.8(3)
N(44)-Na(1)-N(41)-C(412)	138.6(2)
C(42)-Na(1)-N(41)-C(412)	115.5(3)
C(411)-N(41)-C(42)-C(43)	74.9(4)
C(412)-N(41)-C(42)-C(43)	-164.6(3)
Na(1)-N(41)-C(42)-C(43)	-51.2(3)
C(411)-N(41)-C(42)-Na(1)	126.1(3)
C(412)-N(41)-C(42)-Na(1)	-113.4(3)
O(2)-Na(1)-C(42)-N(41)	91.9(2)
N(3)-Na(1)-C(42)-N(41)	-13.7(4)
N(44)-Na(1)-C(42)-N(41)	-150.8(2)
O(2)-Na(1)-C(42)-C(43)	-134.4(2)
N(3)-Na(1)-C(42)-C(43)	120.0(3)
N(41)-Na(1)-C(42)-C(43)	133.8(3)
N(44)-Na(1)-C(42)-C(43)	-17.08(18)
N(41)-C(42)-C(43)-N(44)	62.9(4)
Na(1)-C(42)-C(43)-N(44)	25.6(3)
C(42)-C(43)-N(44)-C(442)	-164.0(3)
C(42)-C(43)-N(44)-C(441)	76.6(4)
C(42)-C(43)-N(44)-Na(1)	-33.3(3)
O(2)-Na(1)-N(44)-C(442)	-131.2(2)
N(3)-Na(1)-N(44)-C(442)	-16.8(3)
N(41)-Na(1)-N(44)-C(442)	128.2(2)
C(42)-Na(1)-N(44)-C(442)	141.5(3)
O(2)-Na(1)-N(44)-C(43)	105.1(2)
N(3)-Na(1)-N(44)-C(43)	-140.5(2)
N(41)-Na(1)-N(44)-C(43)	4.5(2)
C(42)-Na(1)-N(44)-C(43)	17.74(19)
O(2)-Na(1)-N(44)-C(441)	-10.2(2)
N(3)-Na(1)-N(44)-C(441)	104.2(2)
N(41)-Na(1)-N(44)-C(441)	-110.8(2)
C(42)-Na(1)-N(44)-C(441)	-97.6(2)
N(7A)-Zn(2)-C(5)-C(51)	-151.5(8)
C(5A)-Zn(2)-C(5)-C(51)	-63(2)

Electronic Supplementary Information

O(6)-Zn(2)-C(5)-C(51)	45.2(5)
N(7)-Zn(2)-C(5)-C(51)	-135.5(5)
N(7A)-Zn(2)-C(5)-C(53)	88.3(9)
C(5A)-Zn(2)-C(5)-C(53)	177(2)
O(6)-Zn(2)-C(5)-C(53)	-75.0(5)
N(7)-Zn(2)-C(5)-C(53)	104.3(6)
N(7A)-Zn(2)-C(5)-C(52)	-33.2(11)
C(5A)-Zn(2)-C(5)-C(52)	55(2)
O(6)-Zn(2)-C(5)-C(52)	163.5(8)
N(7)-Zn(2)-C(5)-C(52)	-17.2(10)
N(7A)-Zn(2)-O(6)-C(61)	-170.6(5)
C(5A)-Zn(2)-O(6)-C(61)	14.8(5)
C(5)-Zn(2)-O(6)-C(61)	0.0(3)
N(7)-Zn(2)-O(6)-C(61)	-179.7(3)
N(7A)-Zn(2)-O(6)-Na(2)	9.6(4)
C(5A)-Zn(2)-O(6)-Na(2)	-165.0(4)
C(5)-Zn(2)-O(6)-Na(2)	-179.81(18)
N(7)-Zn(2)-O(6)-Na(2)	0.54(18)
N(7)-Na(2)-O(6)-C(61)	179.8(3)
N(81)-Na(2)-O(6)-C(61)	40.1(3)
N(7A)-Na(2)-O(6)-C(61)	173.2(4)
N(84)-Na(2)-O(6)-C(61)	-45.7(3)
C(83)-Na(2)-O(6)-C(61)	-15.2(3)
N(7)-Na(2)-O(6)-Zn(2)	-0.47(15)
N(81)-Na(2)-O(6)-Zn(2)	-140.16(10)
N(7A)-Na(2)-O(6)-Zn(2)	-7.0(3)
N(84)-Na(2)-O(6)-Zn(2)	134.10(11)
C(83)-Na(2)-O(6)-Zn(2)	164.52(12)
Zn(2)-O(6)-C(61)-C(62)	83.9(4)
Na(2)-O(6)-C(61)-C(62)	-96.4(4)
Zn(2)-O(6)-C(61)-C(613)	-97.4(3)
Na(2)-O(6)-C(61)-C(613)	82.2(4)
O(6)-C(61)-C(62)-C(63)	-4.5(6)
C(613)-C(61)-C(62)-C(63)	176.7(4)
O(6)-C(61)-C(62)-C(67)	178.5(3)
C(613)-C(61)-C(62)-C(67)	-0.3(4)
C(61)-C(62)-C(63)-C(64)	-177.8(4)
C(67)-C(62)-C(63)-C(64)	-1.0(5)

Electronic Supplementary Information

C(62)-C(63)-C(64)-C(65)	-2.3(6)
C(63)-C(64)-C(65)-C(66)	5.6(5)
C(63)-C(64)-C(65)-C(60)	-120.9(4)
C(64)-C(65)-C(66)-C(67)	-6.2(5)
C(60)-C(65)-C(66)-C(67)	121.2(4)
C(65)-C(66)-C(67)-C(62)	3.8(6)
C(65)-C(66)-C(67)-C(68)	-178.8(3)
C(61)-C(62)-C(67)-C(66)	177.8(3)
C(63)-C(62)-C(67)-C(66)	0.2(5)
C(61)-C(62)-C(67)-C(68)	-0.2(4)
C(63)-C(62)-C(67)-C(68)	-177.7(3)
C(66)-C(67)-C(68)-C(69)	2.9(6)
C(62)-C(67)-C(68)-C(69)	-179.3(3)
C(66)-C(67)-C(68)-C(613)	-177.1(4)
C(62)-C(67)-C(68)-C(613)	0.6(3)
C(613)-C(68)-C(69)-C(610)	0.7(5)
C(67)-C(68)-C(69)-C(610)	-179.3(3)
C(68)-C(69)-C(610)-C(611)	1.1(5)
C(69)-C(610)-C(611)-C(612)	-1.5(5)
C(610)-C(611)-C(612)-C(613)	0.0(5)
C(611)-C(612)-C(613)-C(68)	1.8(5)
C(611)-C(612)-C(613)-C(61)	-179.9(3)
C(69)-C(68)-C(613)-C(612)	-2.2(5)
C(67)-C(68)-C(613)-C(612)	177.9(3)
C(69)-C(68)-C(613)-C(61)	179.1(3)
C(67)-C(68)-C(613)-C(61)	-0.8(3)
O(6)-C(61)-C(613)-C(612)	3.4(5)
C(62)-C(61)-C(613)-C(612)	-177.7(3)
O(6)-C(61)-C(613)-C(68)	-178.2(3)
C(62)-C(61)-C(613)-C(68)	0.7(4)
C(66)-C(65)-C(60)-C(616)	59.4(4)
C(64)-C(65)-C(60)-C(616)	-174.3(3)
C(66)-C(65)-C(60)-C(615)	179.7(3)
C(64)-C(65)-C(60)-C(615)	-54.0(4)
C(66)-C(65)-C(60)-C(614)	-60.1(4)
C(64)-C(65)-C(60)-C(614)	66.2(4)
N(7A)-Zn(2)-N(7)-C(71)	9(6)
C(5A)-Zn(2)-N(7)-C(71)	-82.1(8)

Electronic Supplementary Information

C(5)-Zn(2)-N(7)-C(71)	-59.6(8)
O(6)-Zn(2)-N(7)-C(71)	119.8(6)
N(7A)-Zn(2)-N(7)-C(75)	140(7)
C(5A)-Zn(2)-N(7)-C(75)	48.8(10)
C(5)-Zn(2)-N(7)-C(75)	71.3(7)
O(6)-Zn(2)-N(7)-C(75)	-109.3(6)
N(7A)-Zn(2)-N(7)-Na(2)	-112(7)
C(5A)-Zn(2)-N(7)-Na(2)	157.6(6)
C(5)-Zn(2)-N(7)-Na(2)	-179.9(4)
O(6)-Zn(2)-N(7)-Na(2)	-0.51(17)
O(6)-Na(2)-N(7)-C(71)	-109.9(4)
N(81)-Na(2)-N(7)-C(71)	1.4(6)
N(7A)-Na(2)-N(7)-C(71)	-65(3)
N(84)-Na(2)-N(7)-C(71)	126.5(4)
C(83)-Na(2)-N(7)-C(71)	110.7(5)
O(6)-Na(2)-N(7)-C(75)	115.5(5)
N(81)-Na(2)-N(7)-C(75)	-133.2(4)
N(7A)-Na(2)-N(7)-C(75)	160(4)
N(84)-Na(2)-N(7)-C(75)	-8.1(6)
C(83)-Na(2)-N(7)-C(75)	-23.8(9)
O(6)-Na(2)-N(7)-Zn(2)	0.46(15)
N(81)-Na(2)-N(7)-Zn(2)	111.8(3)
N(7A)-Na(2)-N(7)-Zn(2)	45(4)
N(84)-Na(2)-N(7)-Zn(2)	-123.12(17)
C(83)-Na(2)-N(7)-Zn(2)	-138.9(5)
C(75)-N(7)-C(71)-C(72)	-45.5(9)
Zn(2)-N(7)-C(71)-C(72)	84.0(6)
Na(2)-N(7)-C(71)-C(72)	-176.0(4)
C(75)-N(7)-C(71)-C(711)	-165.8(6)
Zn(2)-N(7)-C(71)-C(711)	-36.3(7)
Na(2)-N(7)-C(71)-C(711)	63.7(6)
C(75)-N(7)-C(71)-C(712)	83.3(9)
Zn(2)-N(7)-C(71)-C(712)	-147.2(5)
Na(2)-N(7)-C(71)-C(712)	-47.2(6)
N(7)-C(71)-C(72)-C(73)	50.5(6)
C(711)-C(71)-C(72)-C(73)	170.9(4)
C(712)-C(71)-C(72)-C(73)	-78.1(7)
C(71)-C(72)-C(73)-C(74)	-54.1(6)

Electronic Supplementary Information

C(72)-C(73)-C(74)-C(75)	53.4(7)
C(71)-N(7)-C(75)-C(752)	166.2(7)
Zn(2)-N(7)-C(75)-C(752)	39.7(8)
Na(2)-N(7)-C(75)-C(752)	-58.0(6)
C(71)-N(7)-C(75)-C(751)	-80.2(9)
Zn(2)-N(7)-C(75)-C(751)	153.3(5)
Na(2)-N(7)-C(75)-C(751)	55.6(6)
C(71)-N(7)-C(75)-C(74)	43.9(9)
Zn(2)-N(7)-C(75)-C(74)	-82.6(6)
Na(2)-N(7)-C(75)-C(74)	179.7(4)
C(73)-C(74)-C(75)-N(7)	-46.4(7)
C(73)-C(74)-C(75)-C(752)	-167.6(5)
C(73)-C(74)-C(75)-C(751)	78.7(6)
C(5A)-Zn(2)-N(7A)-C(100)	-85.9(18)
C(5)-Zn(2)-N(7A)-C(100)	-63(2)
O(6)-Zn(2)-N(7A)-C(100)	102.0(18)
N(7)-Zn(2)-N(7A)-C(100)	172(8)
C(5A)-Zn(2)-N(7A)-C(104)	58.7(18)
C(5)-Zn(2)-N(7A)-C(104)	81.9(13)
O(6)-Zn(2)-N(7A)-C(104)	-113.3(14)
N(7)-Zn(2)-N(7A)-C(104)	-43(5)
C(5A)-Zn(2)-N(7A)-Na(2)	163.6(7)
C(5)-Zn(2)-N(7A)-Na(2)	-173.3(4)
O(6)-Zn(2)-N(7A)-Na(2)	-8.5(4)
N(7)-Zn(2)-N(7A)-Na(2)	61(6)
O(6)-Na(2)-N(7A)-C(100)	-116.8(8)
N(7)-Na(2)-N(7A)-C(100)	109(4)
N(81)-Na(2)-N(7A)-C(100)	-12.9(12)
N(84)-Na(2)-N(7A)-C(100)	123.1(6)
C(83)-Na(2)-N(7A)-C(100)	102.4(16)
O(6)-Na(2)-N(7A)-C(104)	120.0(9)
N(7)-Na(2)-N(7A)-C(104)	-14(3)
N(81)-Na(2)-N(7A)-C(104)	-136.0(6)
N(84)-Na(2)-N(7A)-C(104)	-0.1(13)
C(83)-Na(2)-N(7A)-C(104)	-21(3)
O(6)-Na(2)-N(7A)-Zn(2)	7.9(3)
N(7)-Na(2)-N(7A)-Zn(2)	-126(4)
N(81)-Na(2)-N(7A)-Zn(2)	111.9(5)

Electronic Supplementary Information

N(84)-Na(2)-N(7A)-Zn(2)	-112.1(5)
C(83)-Na(2)-N(7A)-Zn(2)	-132.8(16)
C(104)-N(7A)-C(100)-C(106)	171.3(16)
Zn(2)-N(7A)-C(100)-C(106)	-46(2)
Na(2)-N(7A)-C(100)-C(106)	57.0(11)
C(104)-N(7A)-C(100)-C(105)	-70(2)
Zn(2)-N(7A)-C(100)-C(105)	73.0(18)
Na(2)-N(7A)-C(100)-C(105)	175.9(8)
C(104)-N(7A)-C(100)-C(101)	47(2)
Zn(2)-N(7A)-C(100)-C(101)	-170.5(16)
Na(2)-N(7A)-C(100)-C(101)	-67.7(12)
N(7A)-C(100)-C(101)-C(102)	-44(2)
C(106)-C(100)-C(101)-C(102)	-164.0(14)
C(105)-C(100)-C(101)-C(102)	77.2(18)
C(100)-C(101)-C(102)-C(103)	51(2)
C(101)-C(102)-C(103)-C(104)	-54.6(15)
C(100)-N(7A)-C(104)-C(103)	-53(2)
Zn(2)-N(7A)-C(104)-C(103)	159.8(11)
Na(2)-N(7A)-C(104)-C(103)	62.9(10)
C(100)-N(7A)-C(104)-C(107)	177.4(16)
Zn(2)-N(7A)-C(104)-C(107)	30.4(17)
Na(2)-N(7A)-C(104)-C(107)	-66.6(11)
C(100)-N(7A)-C(104)-C(108)	66(2)
Zn(2)-N(7A)-C(104)-C(108)	-81.5(13)
Na(2)-N(7A)-C(104)-C(108)	-178.5(6)
C(102)-C(103)-C(104)-N(7A)	52.5(15)
C(102)-C(103)-C(104)-C(107)	176.3(11)
C(102)-C(103)-C(104)-C(108)	-69.7(11)
O(6)-Na(2)-N(81)-C(812)	113.9(3)
N(7)-Na(2)-N(81)-C(812)	13.3(4)
N(7A)-Na(2)-N(81)-C(812)	25.2(6)
N(84)-Na(2)-N(81)-C(812)	-128.3(3)
C(83)-Na(2)-N(81)-C(812)	-140.6(3)
O(6)-Na(2)-N(81)-C(811)	-5.55(16)
N(7)-Na(2)-N(81)-C(811)	-106.2(3)
N(7A)-Na(2)-N(81)-C(811)	-94.3(6)
N(84)-Na(2)-N(81)-C(811)	112.22(14)
C(83)-Na(2)-N(81)-C(811)	99.93(16)

Electronic Supplementary Information

O(6)-Na(2)-N(81)-C(82)	-122.0(2)
N(7)-Na(2)-N(81)-C(82)	137.4(3)
N(7A)-Na(2)-N(81)-C(82)	149.3(6)
N(84)-Na(2)-N(81)-C(82)	-4.2(2)
C(83)-Na(2)-N(81)-C(82)	-16.5(2)
C(812)-N(81)-C(82)-C(83)	162.7(4)
C(811)-N(81)-C(82)-C(83)	-77.8(4)
Na(2)-N(81)-C(82)-C(83)	32.2(4)
N(81)-C(82)-C(83)-N(84)	-60.9(5)
N(81)-C(82)-C(83)-Na(2)	-24.0(3)
O(6)-Na(2)-C(83)-C(82)	113.6(3)
N(7)-Na(2)-C(83)-C(82)	-111.4(6)
N(81)-Na(2)-C(83)-C(82)	16.4(2)
N(7A)-Na(2)-C(83)-C(82)	-108.5(18)
N(84)-Na(2)-C(83)-C(82)	-137.1(4)
O(6)-Na(2)-C(83)-N(84)	-109.3(2)
N(7)-Na(2)-C(83)-N(84)	25.7(7)
N(81)-Na(2)-C(83)-N(84)	153.4(3)
N(7A)-Na(2)-C(83)-N(84)	28.5(18)
C(82)-C(83)-N(84)-C(841)	-76.9(4)
Na(2)-C(83)-N(84)-C(841)	-125.0(3)
C(82)-C(83)-N(84)-C(842)	164.4(4)
Na(2)-C(83)-N(84)-C(842)	116.2(3)
C(82)-C(83)-N(84)-Na(2)	48.1(4)
O(6)-Na(2)-N(84)-C(841)	-154.1(3)
N(7)-Na(2)-N(84)-C(841)	-46.9(4)
N(81)-Na(2)-N(84)-C(841)	99.9(3)
N(7A)-Na(2)-N(84)-C(841)	-49.9(7)
C(83)-Na(2)-N(84)-C(841)	120.8(4)
O(6)-Na(2)-N(84)-C(842)	-27.8(3)
N(7)-Na(2)-N(84)-C(842)	79.4(4)
N(81)-Na(2)-N(84)-C(842)	-133.8(3)
N(7A)-Na(2)-N(84)-C(842)	76.4(7)
C(83)-Na(2)-N(84)-C(842)	-112.8(4)
O(6)-Na(2)-N(84)-C(83)	85.0(2)
N(7)-Na(2)-N(84)-C(83)	-167.7(3)
N(81)-Na(2)-N(84)-C(83)	-20.9(2)
N(7A)-Na(2)-N(84)-C(83)	-170.7(7)

N(7A)-Zn(2)-C(5A)-C(52A)	-111.6(12)
C(5)-Zn(2)-C(5A)-C(52A)	138(3)
O(6)-Zn(2)-C(5A)-C(52A)	59.5(10)
N(7)-Zn(2)-C(5A)-C(52A)	-95.5(11)
N(7A)-Zn(2)-C(5A)-C(53A)	23(2)
C(5)-Zn(2)-C(5A)-C(53A)	-88(3)
O(6)-Zn(2)-C(5A)-C(53A)	-166.0(18)
N(7)-Zn(2)-C(5A)-C(53A)	39(2)
N(7A)-Zn(2)-C(5A)-C(51A)	129.5(10)
C(5)-Zn(2)-C(5A)-C(51A)	18.7(17)
O(6)-Zn(2)-C(5A)-C(51A)	-59.5(9)
N(7)-Zn(2)-C(5A)-C(51A)	145.6(8)

Symmetry transformations used to generate equivalent atoms:

Selected bond distances (Å) and angles (°) for **3**: Na1-O3, 2.2585(13); Na1-N4, 2.4482(16); Na1-N51 2.53(2); Na1-N54, 2.54(2); Zn1-O3, 2.1041(12); Zn1-N4, 2.0121(14); Zn1-C1, 2.0438(18); Zn1-N21; 2.1938(18); Na1-N4-Zn1, 88.05(6); N4-Zn1-O3, 96.27(5); Zn1-O3-Na1, 91.08(5); N51-Na1-N54, 74.5(2); N51-Na1-N4, 136.77(18); N51-Na1-O3, 118.8(3); N54-Na1-N4, 134.3(2); N54-Na1-O3, 117.7(2); N4-Na1-O3, 81.19(5) N4-Zn1-C1, 138.57(7); N4-Zn1-O3, 96.27(5); O3-Zn1-C1, 111.79(6); N21-Zn1-O3, 78.16(5); N21-Zn1-N4, 116.39(6); N21-Zn1-C1, 99.30(6).

Full X-ray data for **3**

Table 1. Crystal data and structure refinement for jksamboth.

Identification code	jksam1	
Empirical formula	C35 H61 N4 Na O Zn	
Formula weight	642.24	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 12.4016(4) Å	α= 90°.
	b = 17.0724(5) Å	β= 92.959(3)°.
	c = 17.6812(5) Å	γ = 90°.
Volume	3738.56(19) Å^3	
Z	4	
Density (calculated)	1.141 Mg/m^3	
Absorption coefficient	0.698 mm^{-1}	

Electronic Supplementary Information

F(000)	1392
Crystal size	0.2 x 0.2 x 0.1 mm^3
Theta range for data collection	2.65 to 27.00°.
Index ranges	-15<=h<=15, -21<=k<=15, -22<=l<=22
Reflections collected	22100
Independent reflections	8152 [R(int) = 0.0338]
Completeness to theta = 27.00°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.95703
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8152 / 128 / 419
Goodness-of-fit on F^2	0.897
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.0697
R indices (all data)	R1 = 0.0614, wR2 = 0.0733
Largest diff. peak and hole	0.415 and -0.436 e.$Å^{-3}$

Electronic Supplementary Information

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

	x	y	z	U(eq)
Na(1)	5219(1)	9648(1)	2500(1)	24(1)
Zn(1)	5544(1)	7857(1)	2259(1)	19(1)
C(1)	4936(2)	7032(1)	1517(1)	25(1)
C(11)	3806(2)	6817(1)	1759(1)	41(1)
C(12)	4837(2)	7242(1)	674(1)	36(1)
C(13)	5631(2)	6295(1)	1591(1)	31(1)
N(21)	5301(1)	7245(1)	3327(1)	19(1)
C(22)	4340(2)	7518(1)	3624(1)	20(1)
C(23)	3821(2)	7011(1)	4150(1)	25(1)
C(24)	4326(2)	6388(1)	4457(1)	25(1)
C(25)	5490(2)	6229(1)	4342(1)	20(1)
C(26)	5794(2)	6653(1)	3635(1)	20(1)
C(20)	6266(2)	6441(1)	5040(1)	24(1)
C(201)	6176(2)	7311(1)	5228(1)	40(1)
C(202)	5941(2)	5961(1)	5724(1)	36(1)
C(203)	7424(2)	6248(1)	4874(1)	32(1)
O(3)	4313(1)	8529(1)	2716(1)	22(1)
C(30)	3904(2)	8190(1)	3296(1)	21(1)
C(31)	2946(2)	8586(1)	3598(1)	23(1)
C(32)	2207(2)	8954(1)	3101(1)	32(1)
C(33)	1350(2)	9373(1)	3366(1)	48(1)
C(34)	1216(2)	9425(1)	4134(1)	51(1)
C(35)	1936(2)	9065(1)	4634(1)	45(1)
C(36)	2802(2)	8653(1)	4370(1)	33(1)
N(4)	6667(1)	8709(1)	2293(1)	20(1)
C(41)	7122(2)	8822(1)	1538(1)	24(1)
C(411)	7653(2)	8082(1)	1220(1)	31(1)
C(412)	6188(2)	9056(1)	990(1)	31(1)
C(42)	7948(2)	9496(1)	1544(1)	29(1)
C(43)	8812(2)	9429(1)	2169(1)	30(1)
C(44)	8266(2)	9396(1)	2917(1)	28(1)
C(45)	7451(2)	8719(1)	2957(1)	23(1)
C(451)	8085(2)	7944(1)	3085(1)	30(1)

Electronic Supplementary Information

C(452)	6814(2)	8865(1)	3667(1)	26(1)
N(51)	4953(9)	10812(9)	3354(9)	29(1)
N(54)	4209(9)	10653(9)	1671(8)	23(1)
C(511)	4228(9)	10503(7)	3909(5)	43(2)
C(512)	5929(12)	11128(11)	3746(6)	41(2)
C(52)	4433(4)	11428(3)	2872(3)	35(1)
C(53)	3645(4)	11062(3)	2272(3)	35(1)
C(541)	3466(10)	10187(6)	1187(5)	45(1)
C(542)	4860(20)	11196(16)	1231(10)	43(2)
N(51A)	4873(9)	10686(9)	3401(9)	29(1)
N(54A)	4397(9)	10771(9)	1748(8)	23(1)
C(53A)	4108(4)	11404(3)	2266(3)	35(1)
C(52A)	3981(4)	11156(3)	3046(2)	35(1)
C(513)	4522(9)	10422(7)	4134(5)	43(2)
C(514)	5854(12)	11165(11)	3512(6)	41(2)
C(543)	3428(10)	10356(6)	1450(4)	45(1)
C(544)	4830(20)	11150(16)	1081(10)	43(2)

Table 3. Bond lengths [Å] and angles [°] for jksamboth.

Na(1)-O(3)	2.2585(13)
Na(1)-N(51A)	2.44(2)
Na(1)-N(4)	2.4482(16)
Na(1)-N(54A)	2.52(2)
Na(1)-N(51)	2.53(2)
Na(1)-N(54)	2.54(2)
Na(1)-C(452)	3.088(2)
Na(1)-Zn(1)	3.1157(7)
Na(1)-C(53)	3.118(5)
Zn(1)-N(4)	2.0121(14)
Zn(1)-C(1)	2.0438(18)
Zn(1)-O(3)	2.1041(12)
Zn(1)-N(21)	2.1938(13)
C(1)-C(13)	1.527(3)
C(1)-C(12)	1.531(2)
C(1)-C(11)	1.531(3)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
N(21)-C(26)	1.286(2)
N(21)-C(22)	1.406(2)
C(22)-C(30)	1.383(2)
C(22)-C(23)	1.445(2)
C(23)-C(24)	1.334(2)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.493(3)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.511(2)
C(25)-C(20)	1.567(2)
C(25)-H(25A)	1.0000

Electronic Supplementary Information

C(26)-H(26A)	0.9500
C(20)-C(203)	1.517(3)
C(20)-C(201)	1.528(2)
C(20)-C(202)	1.532(2)
C(201)-H(20A)	0.9800
C(201)-H(20B)	0.9800
C(201)-H(20C)	0.9800
C(202)-H(20D)	0.9800
C(202)-H(20E)	0.9800
C(202)-H(20F)	0.9800
C(203)-H(20G)	0.9800
C(203)-H(20H)	0.9800
C(203)-H(20I)	0.9800
O(3)-C(30)	1.3042(19)
C(30)-C(31)	1.490(2)
C(31)-C(32)	1.387(3)
C(31)-C(36)	1.391(2)
C(32)-C(33)	1.383(3)
C(32)-H(32A)	0.9500
C(33)-C(34)	1.380(3)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.368(3)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.385(3)
C(35)-H(35A)	0.9500
C(36)-H(36A)	0.9500
N(4)-C(45)	1.485(2)
N(4)-C(41)	1.489(2)
C(41)-C(412)	1.526(3)
C(41)-C(42)	1.540(3)
C(41)-C(411)	1.544(2)
C(411)-H(41A)	0.9800
C(411)-H(41B)	0.9800
C(411)-H(41C)	0.9800
C(412)-H(41D)	0.9800
C(412)-H(41E)	0.9800
C(412)-H(41F)	0.9800
C(42)-C(43)	1.504(3)

Electronic Supplementary Information

C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(44)	1.516(2)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-C(45)	1.541(3)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(452)	1.537(2)
C(45)-C(451)	1.550(2)
C(451)-H(45A)	0.9800
C(451)-H(45B)	0.9800
C(451)-H(45C)	0.9800
C(452)-H(45D)	0.9800
C(452)-H(45E)	0.9800
C(452)-H(45F)	0.9800
N(51)-C(511)	1.461(8)
N(51)-C(512)	1.467(8)
N(51)-C(52)	1.481(8)
N(54)-C(541)	1.460(7)
N(54)-C(542)	1.474(8)
N(54)-C(53)	1.477(8)
C(511)-H(51A)	0.9800
C(511)-H(51B)	0.9800
C(511)-H(51C)	0.9800
C(512)-H(51D)	0.9800
C(512)-H(51E)	0.9800
C(512)-H(51F)	0.9800
C(52)-C(53)	1.537(6)
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(541)-H(54A)	0.9800
C(541)-H(54B)	0.9800
C(541)-H(54C)	0.9800
C(542)-H(54D)	0.9800
C(542)-H(54E)	0.9800

Electronic Supplementary Information

C(542)-H(54F)	0.9800
N(51A)-C(513)	1.459(8)
N(51A)-C(514)	1.470(8)
N(51A)-C(52A)	1.480(8)
N(54A)-C(543)	1.470(7)
N(54A)-C(544)	1.470(8)
N(54A)-C(53A)	1.473(8)
C(53A)-C(52A)	1.459(5)
C(53A)-H(53C)	0.9900
C(53A)-H(53D)	0.9900
C(52A)-H(52C)	0.9900
C(52A)-H(52D)	0.9900
C(513)-H(51G)	0.9800
C(513)-H(51H)	0.9800
C(513)-H(51I)	0.9800
C(514)-H(51J)	0.9800
C(514)-H(51K)	0.9800
C(514)-H(51L)	0.9800
C(543)-H(54G)	0.9800
C(543)-H(54H)	0.9800
C(543)-H(54I)	0.9800
C(544)-H(54J)	0.9800
C(544)-H(54K)	0.9800
C(544)-H(54L)	0.9800

O(3)-Na(1)-N(51A)	113.5(3)
O(3)-Na(1)-N(4)	81.19(5)
N(51A)-Na(1)-N(4)	136.8(2)
O(3)-Na(1)-N(54A)	122.8(2)
N(51A)-Na(1)-N(54A)	73.2(3)
N(4)-Na(1)-N(54A)	134.4(2)
O(3)-Na(1)-N(51)	118.8(3)
N(51A)-Na(1)-N(51)	5.4(5)
N(4)-Na(1)-N(51)	136.3(2)
N(54A)-Na(1)-N(51)	69.8(3)
O(3)-Na(1)-N(54)	115.7(2)
N(51A)-Na(1)-N(54)	77.8(3)
N(4)-Na(1)-N(54)	134.3(2)

N(54A)-Na(1)-N(54)	7.5(4)
N(51)-Na(1)-N(54)	74.8(3)
O(3)-Na(1)-C(452)	80.11(5)
N(51A)-Na(1)-C(452)	90.4(2)
N(4)-Na(1)-C(452)	50.71(5)
N(54A)-Na(1)-C(452)	155.5(2)
N(51)-Na(1)-C(452)	92.3(2)
N(54)-Na(1)-C(452)	163.0(2)
O(3)-Na(1)-Zn(1)	42.47(3)
N(51A)-Na(1)-Zn(1)	146.2(2)
N(4)-Na(1)-Zn(1)	40.20(3)
N(54A)-Na(1)-Zn(1)	136.62(18)
N(51)-Na(1)-Zn(1)	151.0(2)
N(54)-Na(1)-Zn(1)	130.28(17)
C(452)-Na(1)-Zn(1)	65.38(4)
O(3)-Na(1)-C(53)	111.27(10)
N(51A)-Na(1)-C(53)	52.5(2)
N(4)-Na(1)-C(53)	161.23(10)
N(54A)-Na(1)-C(53)	26.9(3)
N(51)-Na(1)-C(53)	50.8(2)
N(54)-Na(1)-C(53)	27.96(19)
C(452)-Na(1)-C(53)	142.84(9)
Zn(1)-Na(1)-C(53)	145.75(9)
N(4)-Zn(1)-C(1)	138.57(7)
N(4)-Zn(1)-O(3)	96.27(5)
C(1)-Zn(1)-O(3)	111.79(6)
N(4)-Zn(1)-N(21)	116.39(6)
C(1)-Zn(1)-N(21)	99.30(6)
O(3)-Zn(1)-N(21)	78.16(5)
N(4)-Zn(1)-Na(1)	51.75(4)
C(1)-Zn(1)-Na(1)	135.92(5)
O(3)-Zn(1)-Na(1)	46.45(3)
N(21)-Zn(1)-Na(1)	109.01(4)
C(13)-C(1)-C(12)	107.10(15)
C(13)-C(1)-C(11)	107.45(16)
C(12)-C(1)-C(11)	107.44(17)
C(13)-C(1)-Zn(1)	108.94(12)
C(12)-C(1)-Zn(1)	118.11(13)

C(11)-C(1)-Zn(1)	107.37(12)
C(1)-C(11)-H(11A)	109.5
C(1)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(1)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(1)-C(12)-H(12A)	109.5
C(1)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(1)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(1)-C(13)-H(13A)	109.5
C(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(26)-N(21)-C(22)	119.77(15)
C(26)-N(21)-Zn(1)	130.86(12)
C(22)-N(21)-Zn(1)	108.68(10)
C(30)-C(22)-N(21)	116.04(15)
C(30)-C(22)-C(23)	126.10(17)
N(21)-C(22)-C(23)	117.09(15)
C(24)-C(23)-C(22)	121.56(18)
C(24)-C(23)-H(23A)	119.2
C(22)-C(23)-H(23A)	119.2
C(23)-C(24)-C(25)	121.78(17)
C(23)-C(24)-H(24A)	119.1
C(25)-C(24)-H(24A)	119.1
C(24)-C(25)-C(26)	108.01(15)
C(24)-C(25)-C(20)	114.24(14)
C(26)-C(25)-C(20)	111.79(15)
C(24)-C(25)-H(25A)	107.5
C(26)-C(25)-H(25A)	107.5
C(20)-C(25)-H(25A)	107.5
N(21)-C(26)-C(25)	126.34(16)

N(21)-C(26)-H(26A)	116.8
C(25)-C(26)-H(26A)	116.8
C(203)-C(20)-C(201)	109.53(17)
C(203)-C(20)-C(202)	109.06(16)
C(201)-C(20)-C(202)	108.83(16)
C(203)-C(20)-C(25)	110.30(14)
C(201)-C(20)-C(25)	110.33(15)
C(202)-C(20)-C(25)	108.76(15)
C(20)-C(201)-H(20A)	109.5
C(20)-C(201)-H(20B)	109.5
H(20A)-C(201)-H(20B)	109.5
C(20)-C(201)-H(20C)	109.5
H(20A)-C(201)-H(20C)	109.5
H(20B)-C(201)-H(20C)	109.5
C(20)-C(202)-H(20D)	109.5
C(20)-C(202)-H(20E)	109.5
H(20D)-C(202)-H(20E)	109.5
C(20)-C(202)-H(20F)	109.5
H(20D)-C(202)-H(20F)	109.5
H(20E)-C(202)-H(20F)	109.5
C(20)-C(203)-H(20G)	109.5
C(20)-C(203)-H(20H)	109.5
H(20G)-C(203)-H(20H)	109.5
C(20)-C(203)-H(20I)	109.5
H(20G)-C(203)-H(20I)	109.5
H(20H)-C(203)-H(20I)	109.5
C(30)-O(3)-Zn(1)	112.27(11)
C(30)-O(3)-Na(1)	136.54(11)
Zn(1)-O(3)-Na(1)	91.08(5)
O(3)-C(30)-C(22)	122.64(16)
O(3)-C(30)-C(31)	115.46(15)
C(22)-C(30)-C(31)	121.88(15)
C(32)-C(31)-C(36)	118.11(18)
C(32)-C(31)-C(30)	119.42(16)
C(36)-C(31)-C(30)	122.29(17)
C(33)-C(32)-C(31)	120.88(19)
C(33)-C(32)-H(32A)	119.6
C(31)-C(32)-H(32A)	119.6

C(34)-C(33)-C(32)	120.1(2)
C(34)-C(33)-H(33A)	120.0
C(32)-C(33)-H(33A)	120.0
C(35)-C(34)-C(33)	119.9(2)
C(35)-C(34)-H(34A)	120.0
C(33)-C(34)-H(34A)	120.0
C(34)-C(35)-C(36)	120.2(2)
C(34)-C(35)-H(35A)	119.9
C(36)-C(35)-H(35A)	119.9
C(35)-C(36)-C(31)	120.87(19)
C(35)-C(36)-H(36A)	119.6
C(31)-C(36)-H(36A)	119.6
C(45)-N(4)-C(41)	116.40(15)
C(45)-N(4)-Zn(1)	117.10(10)
C(41)-N(4)-Zn(1)	111.15(11)
C(45)-N(4)-Na(1)	109.25(10)
C(41)-N(4)-Na(1)	111.32(10)
Zn(1)-N(4)-Na(1)	88.05(6)
N(4)-C(41)-C(412)	107.06(15)
N(4)-C(41)-C(42)	111.95(14)
C(412)-C(41)-C(42)	106.94(15)
N(4)-C(41)-C(411)	114.12(14)
C(412)-C(41)-C(411)	107.91(15)
C(42)-C(41)-C(411)	108.53(16)
C(41)-C(411)-H(41A)	109.5
C(41)-C(411)-H(41B)	109.5
H(41A)-C(411)-H(41B)	109.5
C(41)-C(411)-H(41C)	109.5
H(41A)-C(411)-H(41C)	109.5
H(41B)-C(411)-H(41C)	109.5
C(41)-C(412)-H(41D)	109.5
C(41)-C(412)-H(41E)	109.5
H(41D)-C(412)-H(41E)	109.5
C(41)-C(412)-H(41F)	109.5
H(41D)-C(412)-H(41F)	109.5
H(41E)-C(412)-H(41F)	109.5
C(43)-C(42)-C(41)	113.31(15)
C(43)-C(42)-H(42A)	108.9

C(41)-C(42)-H(42A)	108.9
C(43)-C(42)-H(42B)	108.9
C(41)-C(42)-H(42B)	108.9
H(42A)-C(42)-H(42B)	107.7
C(42)-C(43)-C(44)	108.08(16)
C(42)-C(43)-H(43A)	110.1
C(44)-C(43)-H(43A)	110.1
C(42)-C(43)-H(43B)	110.1
C(44)-C(43)-H(43B)	110.1
H(43A)-C(43)-H(43B)	108.4
C(43)-C(44)-C(45)	113.06(15)
C(43)-C(44)-H(44A)	109.0
C(45)-C(44)-H(44A)	109.0
C(43)-C(44)-H(44B)	109.0
C(45)-C(44)-H(44B)	109.0
H(44A)-C(44)-H(44B)	107.8
N(4)-C(45)-C(452)	107.74(15)
N(4)-C(45)-C(44)	112.11(14)
C(452)-C(45)-C(44)	106.40(15)
N(4)-C(45)-C(451)	114.38(14)
C(452)-C(45)-C(451)	107.27(14)
C(44)-C(45)-C(451)	108.54(16)
C(45)-C(451)-H(45A)	109.5
C(45)-C(451)-H(45B)	109.5
H(45A)-C(451)-H(45B)	109.5
C(45)-C(451)-H(45C)	109.5
H(45A)-C(451)-H(45C)	109.5
H(45B)-C(451)-H(45C)	109.5
C(45)-C(452)-Na(1)	82.11(10)
C(45)-C(452)-H(45D)	109.5
Na(1)-C(452)-H(45D)	41.2
C(45)-C(452)-H(45E)	109.5
Na(1)-C(452)-H(45E)	149.8
H(45D)-C(452)-H(45E)	109.5
C(45)-C(452)-H(45F)	109.5
Na(1)-C(452)-H(45F)	91.4
H(45D)-C(452)-H(45F)	109.5
H(45E)-C(452)-H(45F)	109.5

C(511)-N(51)-C(512)	109.7(13)
C(511)-N(51)-C(52)	112.2(8)
C(512)-N(51)-C(52)	109.6(10)
C(511)-N(51)-Na(1)	102.8(10)
C(512)-N(51)-Na(1)	116.2(10)
C(52)-N(51)-Na(1)	106.3(9)
C(541)-N(54)-C(542)	112.2(14)
C(541)-N(54)-C(53)	111.7(6)
C(542)-N(54)-C(53)	111.9(13)
C(541)-N(54)-Na(1)	104.3(10)
C(542)-N(54)-Na(1)	117.6(15)
C(53)-N(54)-Na(1)	98.2(9)
N(51)-C(52)-C(53)	110.6(8)
N(51)-C(52)-H(52A)	109.5
C(53)-C(52)-H(52A)	109.5
N(51)-C(52)-H(52B)	109.5
C(53)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	108.1
N(54)-C(53)-C(52)	112.4(6)
N(54)-C(53)-Na(1)	53.8(8)
C(52)-C(53)-Na(1)	81.6(3)
N(54)-C(53)-H(53A)	109.1
C(52)-C(53)-H(53A)	109.1
Na(1)-C(53)-H(53A)	79.8
N(54)-C(53)-H(53B)	109.1
C(52)-C(53)-H(53B)	109.1
Na(1)-C(53)-H(53B)	162.9
H(53A)-C(53)-H(53B)	107.9
C(513)-N(51A)-C(514)	109.6(13)
C(513)-N(51A)-C(52A)	107.1(8)
C(514)-N(51A)-C(52A)	110.5(10)
C(513)-N(51A)-Na(1)	115.3(10)
C(514)-N(51A)-Na(1)	108.6(10)
C(52A)-N(51A)-Na(1)	105.7(9)
C(543)-N(54A)-C(544)	104.5(15)
C(543)-N(54A)-C(53A)	110.8(7)
C(544)-N(54A)-C(53A)	106.7(13)
C(543)-N(54A)-Na(1)	97.1(10)

C(544)-N(54A)-Na(1)	127.1(15)
C(53A)-N(54A)-Na(1)	109.6(9)
C(52A)-C(53A)-N(54A)	114.6(8)
C(52A)-C(53A)-H(53C)	108.6
N(54A)-C(53A)-H(53C)	108.6
C(52A)-C(53A)-H(53D)	108.6
N(54A)-C(53A)-H(53D)	108.6
H(53C)-C(53A)-H(53D)	107.6
C(53A)-C(52A)-N(51A)	116.3(7)
C(53A)-C(52A)-H(52C)	108.2
N(51A)-C(52A)-H(52C)	108.2
C(53A)-C(52A)-H(52D)	108.2
N(51A)-C(52A)-H(52D)	108.2
H(52C)-C(52A)-H(52D)	107.4
N(51A)-C(513)-H(51G)	109.5
N(51A)-C(513)-H(51H)	109.5
H(51G)-C(513)-H(51H)	109.5
N(51A)-C(513)-H(51I)	109.5
H(51G)-C(513)-H(51I)	109.5
H(51H)-C(513)-H(51I)	109.5
N(51A)-C(514)-H(51J)	109.5
N(51A)-C(514)-H(51K)	109.5
H(51J)-C(514)-H(51K)	109.5
N(51A)-C(514)-H(51L)	109.5
H(51J)-C(514)-H(51L)	109.5
H(51K)-C(514)-H(51L)	109.5
N(54A)-C(543)-H(54G)	109.5
N(54A)-C(543)-H(54H)	109.5
H(54G)-C(543)-H(54H)	109.5
N(54A)-C(543)-H(54I)	109.5
H(54G)-C(543)-H(54I)	109.5
H(54H)-C(543)-H(54I)	109.5
N(54A)-C(544)-H(54J)	109.5
N(54A)-C(544)-H(54K)	109.5
H(54J)-C(544)-H(54K)	109.5
N(54A)-C(544)-H(54L)	109.5
H(54J)-C(544)-H(54L)	109.5
H(54K)-C(544)-H(54L)	109.5

Symmetry transformations used to generate equivalent atoms:

Electronic Supplementary Information

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for jksamboth. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Na(1)	28(1)	21(1)	23(1)	-1(1)	4(1)	3(1)
Zn(1)	21(1)	19(1)	18(1)	0(1)	6(1)	1(1)
C(1)	25(1)	25(1)	25(1)	-3(1)	3(1)	-2(1)
C(11)	31(1)	48(1)	45(1)	-16(1)	5(1)	-12(1)
C(12)	42(1)	35(1)	29(1)	-5(1)	-4(1)	1(1)
C(13)	40(1)	24(1)	28(1)	-4(1)	4(1)	-3(1)
N(21)	20(1)	19(1)	19(1)	-1(1)	3(1)	0(1)
C(22)	19(1)	21(1)	19(1)	-1(1)	5(1)	2(1)
C(23)	20(1)	29(1)	27(1)	2(1)	8(1)	1(1)
C(24)	24(1)	25(1)	26(1)	7(1)	8(1)	-3(1)
C(25)	24(1)	14(1)	22(1)	0(1)	5(1)	0(1)
C(26)	21(1)	20(1)	21(1)	-3(1)	7(1)	-1(1)
C(20)	29(1)	23(1)	21(1)	-1(1)	4(1)	2(1)
C(201)	58(2)	29(1)	32(1)	-9(1)	-9(1)	3(1)
C(202)	36(1)	45(1)	27(1)	8(1)	2(1)	-1(1)
C(203)	29(1)	37(1)	31(1)	-1(1)	-2(1)	-3(1)
O(3)	22(1)	23(1)	20(1)	4(1)	7(1)	2(1)
C(30)	18(1)	23(1)	21(1)	1(1)	3(1)	0(1)
C(31)	19(1)	23(1)	27(1)	6(1)	7(1)	2(1)
C(32)	25(1)	42(1)	29(1)	9(1)	4(1)	4(1)
C(33)	29(1)	65(2)	50(1)	21(1)	5(1)	21(1)
C(34)	40(2)	62(2)	54(2)	18(1)	26(1)	31(1)
C(35)	49(2)	53(2)	35(1)	12(1)	24(1)	21(1)
C(36)	31(1)	40(1)	28(1)	10(1)	9(1)	13(1)
N(4)	22(1)	20(1)	19(1)	0(1)	6(1)	-1(1)
C(41)	29(1)	21(1)	22(1)	1(1)	11(1)	-2(1)
C(411)	37(1)	28(1)	30(1)	-3(1)	16(1)	-3(1)
C(412)	45(1)	28(1)	21(1)	4(1)	9(1)	0(1)
C(42)	38(1)	19(1)	31(1)	2(1)	16(1)	-3(1)
C(43)	28(1)	22(1)	43(1)	0(1)	14(1)	-7(1)
C(44)	25(1)	27(1)	33(1)	-2(1)	4(1)	-5(1)
C(45)	21(1)	22(1)	26(1)	1(1)	2(1)	-1(1)
C(451)	25(1)	28(1)	38(1)	5(1)	2(1)	0(1)

Electronic Supplementary Information

C(452)	28(1)	28(1)	22(1)	1(1)	1(1)	-4(1)
N(51)	34(2)	25(4)	27(2)	-8(2)	-3(1)	4(2)
N(54)	23(3)	27(4)	19(2)	-5(1)	-6(3)	-4(2)
C(511)	57(5)	44(3)	30(5)	-8(3)	7(3)	0(3)
C(512)	45(2)	42(2)	37(6)	-18(5)	-2(4)	1(2)
C(52)	41(3)	34(3)	32(2)	-7(2)	5(2)	11(2)
C(53)	37(3)	29(3)	37(2)	-2(2)	-2(2)	9(2)
C(541)	42(2)	45(4)	44(5)	-3(3)	-18(4)	-10(2)
C(542)	53(2)	39(2)	37(5)	6(4)	-2(5)	-4(2)
N(51A)	34(2)	25(4)	27(2)	-8(2)	-3(1)	4(2)
N(54A)	23(3)	27(4)	19(2)	-5(1)	-6(3)	-4(2)
C(53A)	37(3)	29(3)	37(2)	-2(2)	-2(2)	9(2)
C(52A)	41(3)	34(3)	32(2)	-7(2)	5(2)	11(2)
C(513)	57(5)	44(3)	30(5)	-8(3)	7(3)	0(3)
C(514)	45(2)	42(2)	37(6)	-18(5)	-2(4)	1(2)
C(543)	42(2)	45(4)	44(5)	-3(3)	-18(4)	-10(2)
C(544)	53(2)	39(2)	37(5)	6(4)	-2(5)	-4(2)

Electronic Supplementary Information

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for jksamboth.

	x	y	z	U(eq)
H(11A)	3505	6400	1430	62
H(11B)	3337	7279	1717	62
H(11C)	3851	6634	2285	62
H(12A)	4524	6799	387	53
H(12B)	5554	7361	496	53
H(12C)	4369	7702	601	53
H(13A)	5318	5884	1261	46
H(13B)	5658	6113	2118	46
H(13C)	6364	6414	1443	46
H(23A)	3104	7124	4280	30
H(24A)	3934	6037	4756	30
H(25A)	5565	5654	4247	24
H(26A)	6410	6465	3393	24
H(20A)	6651	7433	5672	60
H(20B)	5428	7435	5336	60
H(20C)	6392	7623	4796	60
H(20D)	6435	6078	6160	54
H(20E)	5978	5402	5604	54
H(20F)	5202	6097	5845	54
H(20G)	7894	6346	5326	48
H(20H)	7652	6577	4457	48
H(20I)	7475	5695	4730	48
H(32A)	2290	8917	2571	38
H(33A)	854	9625	3019	57
H(34A)	624	9710	4316	61
H(35A)	1841	9098	5162	54
H(36A)	3305	8413	4722	39
H(41A)	7168	7634	1267	47
H(41B)	8337	7979	1506	47
H(41C)	7792	8165	686	47
H(41D)	5895	9562	1144	47
H(41E)	5620	8657	995	47

Electronic Supplementary Information

H(41F)	6447	9101	477	47
H(42A)	8293	9506	1051	35
H(42B)	7562	9999	1599	35
H(43A)	9302	9886	2161	36
H(43B)	9243	8948	2101	36
H(44A)	7887	9898	2994	34
H(44B)	8825	9337	3333	34
H(45A)	8503	7833	2642	45
H(45B)	7577	7514	3160	45
H(45C)	8576	7994	3535	45
H(45D)	6405	9353	3606	39
H(45E)	7318	8905	4111	39
H(45F)	6315	8429	3736	39
H(51A)	4577	10062	4180	65
H(51B)	3557	10324	3648	65
H(51C)	4066	10916	4271	65
H(51D)	5742	11594	4035	62
H(51E)	6453	11270	3373	62
H(51F)	6245	10732	4092	62
H(52A)	4993	11729	2618	42
H(52B)	4037	11794	3191	42
H(53A)	3170	10686	2521	42
H(53B)	3183	11479	2040	42
H(54A)	3129	9784	1492	67
H(54B)	3864	9936	789	67
H(54C)	2905	10528	956	67
H(54D)	5220	10903	841	64
H(54E)	5398	11453	1570	64
H(54F)	4382	11592	990	64
H(53C)	4675	11813	2264	42
H(53D)	3423	11645	2070	42
H(52C)	3308	10846	3061	42
H(52D)	3888	11630	3359	42
H(51G)	4403	10878	4457	65
H(51H)	5079	10086	4377	65
H(51I)	3848	10126	4061	65
H(51J)	5692	11632	3807	62
H(51K)	6105	11323	3018	62

H(51L)	6418	10858	3785	62
H(54G)	2961	10721	1157	67
H(54H)	3036	10145	1872	67
H(54I)	3641	9926	1123	67
H(54J)	4962	10753	696	64
H(54K)	5509	11415	1229	64
H(54L)	4308	11534	873	64

Table 6. Torsion angles [°] for jksamboth.

O(3)-Na(1)-Zn(1)-N(4)	-160.27(7)
N(51A)-Na(1)-Zn(1)-N(4)	-105.2(5)
N(54A)-Na(1)-Zn(1)-N(4)	109.0(4)
N(51)-Na(1)-Zn(1)-N(4)	-100.2(5)
N(54)-Na(1)-Zn(1)-N(4)	114.6(3)
C(452)-Na(1)-Zn(1)-N(4)	-57.52(6)
C(53)-Na(1)-Zn(1)-N(4)	150.27(17)
O(3)-Na(1)-Zn(1)-C(1)	75.79(9)
N(51A)-Na(1)-Zn(1)-C(1)	130.8(5)
N(4)-Na(1)-Zn(1)-C(1)	-123.94(9)
N(54A)-Na(1)-Zn(1)-C(1)	-14.9(4)
N(51)-Na(1)-Zn(1)-C(1)	135.9(5)
N(54)-Na(1)-Zn(1)-C(1)	-9.3(3)
C(452)-Na(1)-Zn(1)-C(1)	178.54(8)
C(53)-Na(1)-Zn(1)-C(1)	26.33(18)
N(51A)-Na(1)-Zn(1)-O(3)	55.0(5)
N(4)-Na(1)-Zn(1)-O(3)	160.27(7)
N(54A)-Na(1)-Zn(1)-O(3)	-90.7(4)
N(51)-Na(1)-Zn(1)-O(3)	60.1(5)
N(54)-Na(1)-Zn(1)-O(3)	-85.1(3)
C(452)-Na(1)-Zn(1)-O(3)	102.75(6)
C(53)-Na(1)-Zn(1)-O(3)	-49.46(17)
O(3)-Na(1)-Zn(1)-N(21)	-51.17(6)
N(51A)-Na(1)-Zn(1)-N(21)	3.9(5)
N(4)-Na(1)-Zn(1)-N(21)	109.10(7)
N(54A)-Na(1)-Zn(1)-N(21)	-141.9(4)
N(51)-Na(1)-Zn(1)-N(21)	8.9(5)
N(54)-Na(1)-Zn(1)-N(21)	-136.3(3)
C(452)-Na(1)-Zn(1)-N(21)	51.57(6)
C(53)-Na(1)-Zn(1)-N(21)	-100.63(17)
N(4)-Zn(1)-C(1)-C(13)	86.56(15)
O(3)-Zn(1)-C(1)-C(13)	-144.34(11)
N(21)-Zn(1)-C(1)-C(13)	-63.46(13)
Na(1)-Zn(1)-C(1)-C(13)	166.49(9)
N(4)-Zn(1)-C(1)-C(12)	-35.8(2)
O(3)-Zn(1)-C(1)-C(12)	93.27(15)

Electronic Supplementary Information

N(21)-Zn(1)-C(1)-C(12)	174.15(14)
Na(1)-Zn(1)-C(1)-C(12)	44.10(18)
N(4)-Zn(1)-C(1)-C(11)	-157.37(12)
O(3)-Zn(1)-C(1)-C(11)	-28.27(15)
N(21)-Zn(1)-C(1)-C(11)	52.61(14)
Na(1)-Zn(1)-C(1)-C(11)	-77.43(15)
N(4)-Zn(1)-N(21)-C(26)	-85.81(16)
C(1)-Zn(1)-N(21)-C(26)	72.53(17)
O(3)-Zn(1)-N(21)-C(26)	-176.98(16)
Na(1)-Zn(1)-N(21)-C(26)	-141.75(15)
N(4)-Zn(1)-N(21)-C(22)	103.98(12)
C(1)-Zn(1)-N(21)-C(22)	-97.69(12)
O(3)-Zn(1)-N(21)-C(22)	12.80(11)
Na(1)-Zn(1)-N(21)-C(22)	48.03(11)
C(26)-N(21)-C(22)-C(30)	175.45(16)
Zn(1)-N(21)-C(22)-C(30)	-13.06(18)
C(26)-N(21)-C(22)-C(23)	-14.0(2)
Zn(1)-N(21)-C(22)-C(23)	157.48(13)
C(30)-C(22)-C(23)-C(24)	-177.63(18)
N(21)-C(22)-C(23)-C(24)	12.9(3)
C(22)-C(23)-C(24)-C(25)	6.8(3)
C(23)-C(24)-C(25)-C(26)	-22.0(2)
C(23)-C(24)-C(25)-C(20)	103.1(2)
C(22)-N(21)-C(26)-C(25)	-4.5(3)
Zn(1)-N(21)-C(26)-C(25)	-173.84(12)
C(24)-C(25)-C(26)-N(21)	21.8(2)
C(20)-C(25)-C(26)-N(21)	-104.7(2)
C(24)-C(25)-C(20)-C(203)	179.16(15)
C(26)-C(25)-C(20)-C(203)	-57.80(19)
C(24)-C(25)-C(20)-C(201)	-59.7(2)
C(26)-C(25)-C(20)-C(201)	63.3(2)
C(24)-C(25)-C(20)-C(202)	59.6(2)
C(26)-C(25)-C(20)-C(202)	-177.36(15)
N(4)-Zn(1)-O(3)-C(30)	-126.93(12)
C(1)-Zn(1)-O(3)-C(30)	84.18(13)
N(21)-Zn(1)-O(3)-C(30)	-11.21(11)
Na(1)-Zn(1)-O(3)-C(30)	-142.40(13)
N(4)-Zn(1)-O(3)-Na(1)	15.47(5)

Electronic Supplementary Information

C(1)-Zn(1)-O(3)-Na(1)	-133.43(6)
N(21)-Zn(1)-O(3)-Na(1)	131.18(5)
N(51A)-Na(1)-O(3)-C(30)	-25.4(3)
N(4)-Na(1)-O(3)-C(30)	112.08(17)
N(54A)-Na(1)-O(3)-C(30)	-110.0(3)
N(51)-Na(1)-O(3)-C(30)	-26.5(3)
N(54)-Na(1)-O(3)-C(30)	-112.7(3)
C(452)-Na(1)-O(3)-C(30)	60.65(17)
Zn(1)-Na(1)-O(3)-C(30)	124.82(18)
C(53)-Na(1)-O(3)-C(30)	-82.50(19)
N(51A)-Na(1)-O(3)-Zn(1)	-150.2(2)
N(4)-Na(1)-O(3)-Zn(1)	-12.74(4)
N(54A)-Na(1)-O(3)-Zn(1)	125.2(2)
N(51)-Na(1)-O(3)-Zn(1)	-151.3(2)
N(54)-Na(1)-O(3)-Zn(1)	122.5(2)
C(452)-Na(1)-O(3)-Zn(1)	-64.17(5)
C(53)-Na(1)-O(3)-Zn(1)	152.68(9)
Zn(1)-O(3)-C(30)-C(22)	8.0(2)
Na(1)-O(3)-C(30)-C(22)	-109.52(19)
Zn(1)-O(3)-C(30)-C(31)	-173.47(12)
Na(1)-O(3)-C(30)-C(31)	69.0(2)
N(21)-C(22)-C(30)-O(3)	4.1(3)
C(23)-C(22)-C(30)-O(3)	-165.49(17)
N(21)-C(22)-C(30)-C(31)	-174.37(16)
C(23)-C(22)-C(30)-C(31)	16.1(3)
O(3)-C(30)-C(31)-C(32)	35.5(3)
C(22)-C(30)-C(31)-C(32)	-145.97(19)
O(3)-C(30)-C(31)-C(36)	-139.63(18)
C(22)-C(30)-C(31)-C(36)	38.9(3)
C(36)-C(31)-C(32)-C(33)	-0.2(3)
C(30)-C(31)-C(32)-C(33)	-175.47(19)
C(31)-C(32)-C(33)-C(34)	-0.5(4)
C(32)-C(33)-C(34)-C(35)	0.5(4)
C(33)-C(34)-C(35)-C(36)	0.4(4)
C(34)-C(35)-C(36)-C(31)	-1.1(4)
C(32)-C(31)-C(36)-C(35)	1.0(3)
C(30)-C(31)-C(36)-C(35)	176.14(19)
C(1)-Zn(1)-N(4)-C(45)	-130.03(13)

Electronic Supplementary Information

O(3)-Zn(1)-N(4)-C(45)	96.43(12)
N(21)-Zn(1)-N(4)-C(45)	16.57(14)
Na(1)-Zn(1)-N(4)-C(45)	110.68(13)
C(1)-Zn(1)-N(4)-C(41)	7.15(17)
O(3)-Zn(1)-N(4)-C(41)	-126.39(11)
N(21)-Zn(1)-N(4)-C(41)	153.74(11)
Na(1)-Zn(1)-N(4)-C(41)	-112.14(12)
C(1)-Zn(1)-N(4)-Na(1)	119.29(9)
O(3)-Zn(1)-N(4)-Na(1)	-14.25(5)
N(21)-Zn(1)-N(4)-Na(1)	-94.11(6)
O(3)-Na(1)-N(4)-C(45)	-104.75(11)
N(51A)-Na(1)-N(4)-C(45)	10.3(4)
N(54A)-Na(1)-N(4)-C(45)	127.3(3)
N(51)-Na(1)-N(4)-C(45)	18.2(4)
N(54)-Na(1)-N(4)-C(45)	137.8(3)
C(452)-Na(1)-N(4)-C(45)	-20.37(10)
Zn(1)-Na(1)-N(4)-C(45)	-118.09(12)
C(53)-Na(1)-N(4)-C(45)	122.0(3)
O(3)-Na(1)-N(4)-C(41)	125.31(11)
N(51A)-Na(1)-N(4)-C(41)	-119.6(4)
N(54A)-Na(1)-N(4)-C(41)	-2.7(3)
N(51)-Na(1)-N(4)-C(41)	-111.8(4)
N(54)-Na(1)-N(4)-C(41)	7.9(3)
C(452)-Na(1)-N(4)-C(41)	-150.30(13)
Zn(1)-Na(1)-N(4)-C(41)	111.98(12)
C(53)-Na(1)-N(4)-C(41)	-7.9(3)
O(3)-Na(1)-N(4)-Zn(1)	13.34(5)
N(51A)-Na(1)-N(4)-Zn(1)	128.4(4)
N(54A)-Na(1)-N(4)-Zn(1)	-114.6(3)
N(51)-Na(1)-N(4)-Zn(1)	136.3(3)
N(54)-Na(1)-N(4)-Zn(1)	-104.1(3)
C(452)-Na(1)-N(4)-Zn(1)	97.72(7)
C(53)-Na(1)-N(4)-Zn(1)	-119.9(3)
C(45)-N(4)-C(41)-C(412)	-161.88(14)
Zn(1)-N(4)-C(41)-C(412)	60.62(15)
Na(1)-N(4)-C(41)-C(412)	-35.80(16)
C(45)-N(4)-C(41)-C(42)	-45.0(2)
Zn(1)-N(4)-C(41)-C(42)	177.52(12)

Electronic Supplementary Information

Na(1)-N(4)-C(41)-C(42)	81.10(16)
C(45)-N(4)-C(41)-C(411)	78.8(2)
Zn(1)-N(4)-C(41)-C(411)	-58.71(18)
Na(1)-N(4)-C(41)-C(411)	-155.13(13)
N(4)-C(41)-C(42)-C(43)	51.6(2)
C(412)-C(41)-C(42)-C(43)	168.61(15)
C(411)-C(41)-C(42)-C(43)	-75.21(19)
C(41)-C(42)-C(43)-C(44)	-57.4(2)
C(42)-C(43)-C(44)-C(45)	57.2(2)
C(41)-N(4)-C(45)-C(452)	161.75(13)
Zn(1)-N(4)-C(45)-C(452)	-63.31(16)
Na(1)-N(4)-C(45)-C(452)	34.64(15)
C(41)-N(4)-C(45)-C(44)	45.0(2)
Zn(1)-N(4)-C(45)-C(44)	179.96(11)
Na(1)-N(4)-C(45)-C(44)	-82.10(15)
C(41)-N(4)-C(45)-C(451)	-79.10(19)
Zn(1)-N(4)-C(45)-C(451)	55.85(18)
Na(1)-N(4)-C(45)-C(451)	153.79(12)
C(43)-C(44)-C(45)-N(4)	-51.3(2)
C(43)-C(44)-C(45)-C(452)	-168.89(16)
C(43)-C(44)-C(45)-C(451)	76.0(2)
N(4)-C(45)-C(452)-Na(1)	-25.44(11)
C(44)-C(45)-C(452)-Na(1)	94.97(13)
C(451)-C(45)-C(452)-Na(1)	-149.03(13)
O(3)-Na(1)-C(452)-C(45)	105.35(10)
N(51A)-Na(1)-C(452)-C(45)	-140.9(3)
N(4)-Na(1)-C(452)-C(45)	18.69(9)
N(54A)-Na(1)-C(452)-C(45)	-93.9(6)
N(51)-Na(1)-C(452)-C(45)	-135.8(3)
N(54)-Na(1)-C(452)-C(45)	-95.7(8)
Zn(1)-Na(1)-C(452)-C(45)	63.40(9)
C(53)-Na(1)-C(452)-C(45)	-142.34(18)
O(3)-Na(1)-N(51)-C(511)	2.9(6)
N(51A)-Na(1)-N(51)-C(511)	-8(4)
N(4)-Na(1)-N(51)-C(511)	-105.9(5)
N(54A)-Na(1)-N(51)-C(511)	120.1(6)
N(54)-Na(1)-N(51)-C(511)	114.2(6)
C(452)-Na(1)-N(51)-C(511)	-77.0(5)

Electronic Supplementary Information

Zn(1)-Na(1)-N(51)-C(511)	-39.0(9)
C(53)-Na(1)-N(51)-C(511)	97.9(6)
O(3)-Na(1)-N(51)-C(512)	122.7(7)
N(51A)-Na(1)-N(51)-C(512)	112(5)
N(4)-Na(1)-N(51)-C(512)	13.9(9)
N(54A)-Na(1)-N(51)-C(512)	-120.1(8)
N(54)-Na(1)-N(51)-C(512)	-126.0(8)
C(452)-Na(1)-N(51)-C(512)	42.7(7)
Zn(1)-Na(1)-N(51)-C(512)	80.8(8)
C(53)-Na(1)-N(51)-C(512)	-142.3(8)
O(3)-Na(1)-N(51)-C(52)	-115.1(5)
N(51A)-Na(1)-N(51)-C(52)	-126(5)
N(4)-Na(1)-N(51)-C(52)	136.0(4)
N(54A)-Na(1)-N(51)-C(52)	2.0(6)
N(54)-Na(1)-N(51)-C(52)	-3.9(6)
C(452)-Na(1)-N(51)-C(52)	164.9(6)
Zn(1)-Na(1)-N(51)-C(52)	-157.0(3)
C(53)-Na(1)-N(51)-C(52)	-20.2(4)
O(3)-Na(1)-N(54)-C(541)	-27.7(6)
N(51A)-Na(1)-N(54)-C(541)	-138.1(7)
N(4)-Na(1)-N(54)-C(541)	75.7(6)
N(54A)-Na(1)-N(54)-C(541)	170(4)
N(51)-Na(1)-N(54)-C(541)	-142.8(7)
C(452)-Na(1)-N(54)-C(541)	175.4(5)
Zn(1)-Na(1)-N(54)-C(541)	20.6(7)
C(53)-Na(1)-N(54)-C(541)	-115.0(8)
O(3)-Na(1)-N(54)-C(542)	-152.7(10)
N(51A)-Na(1)-N(54)-C(542)	97.0(11)
N(4)-Na(1)-N(54)-C(542)	-49.3(11)
N(54A)-Na(1)-N(54)-C(542)	45(3)
N(51)-Na(1)-N(54)-C(542)	92.3(10)
C(452)-Na(1)-N(54)-C(542)	50.4(14)
Zn(1)-Na(1)-N(54)-C(542)	-104.4(10)
C(53)-Na(1)-N(54)-C(542)	120.0(11)
O(3)-Na(1)-N(54)-C(53)	87.3(5)
N(51A)-Na(1)-N(54)-C(53)	-23.0(5)
N(4)-Na(1)-N(54)-C(53)	-169.3(3)
N(54A)-Na(1)-N(54)-C(53)	-75(3)

Electronic Supplementary Information

N(51)-Na(1)-N(54)-C(53)	-27.7(5)
C(452)-Na(1)-N(54)-C(53)	-69.6(11)
Zn(1)-Na(1)-N(54)-C(53)	135.6(3)
C(511)-N(51)-C(52)-C(53)	-76.2(14)
C(512)-N(51)-C(52)-C(53)	161.7(11)
Na(1)-N(51)-C(52)-C(53)	35.4(7)
C(541)-N(54)-C(53)-C(52)	169.3(10)
C(542)-N(54)-C(53)-C(52)	-63.9(17)
Na(1)-N(54)-C(53)-C(52)	60.2(6)
C(541)-N(54)-C(53)-Na(1)	109.1(14)
C(542)-N(54)-C(53)-Na(1)	-124.2(16)
N(51)-C(52)-C(53)-N(54)	-72.3(11)
N(51)-C(52)-C(53)-Na(1)	-27.1(6)
O(3)-Na(1)-C(53)-N(54)	-104.9(5)
N(51A)-Na(1)-C(53)-N(54)	151.2(6)
N(4)-Na(1)-C(53)-N(54)	24.5(6)
N(54A)-Na(1)-C(53)-N(54)	16.2(9)
N(51)-Na(1)-C(53)-N(54)	144.6(6)
C(452)-Na(1)-C(53)-N(54)	153.0(5)
Zn(1)-Na(1)-C(53)-N(54)	-71.5(5)
O(3)-Na(1)-C(53)-C(52)	129.3(3)
N(51A)-Na(1)-C(53)-C(52)	25.4(4)
N(4)-Na(1)-C(53)-C(52)	-101.3(3)
N(54A)-Na(1)-C(53)-C(52)	-109.6(6)
N(51)-Na(1)-C(53)-C(52)	18.8(4)
N(54)-Na(1)-C(53)-C(52)	-125.8(6)
C(452)-Na(1)-C(53)-C(52)	27.3(4)
Zn(1)-Na(1)-C(53)-C(52)	162.7(2)
O(3)-Na(1)-N(51A)-C(513)	24.4(7)
N(4)-Na(1)-N(51A)-C(513)	-78.2(8)
N(54A)-Na(1)-N(51A)-C(513)	143.5(8)
N(51)-Na(1)-N(51A)-C(513)	-166(5)
N(54)-Na(1)-N(51A)-C(513)	137.3(7)
C(452)-Na(1)-N(51A)-C(513)	-54.9(7)
Zn(1)-Na(1)-N(51A)-C(513)	-12.7(10)
C(53)-Na(1)-N(51A)-C(513)	123.9(8)
O(3)-Na(1)-N(51A)-C(514)	147.9(6)
N(4)-Na(1)-N(51A)-C(514)	45.2(8)

Electronic Supplementary Information

N(54A)-Na(1)-N(51A)-C(514)	-93.1(7)
N(51)-Na(1)-N(51A)-C(514)	-42(5)
N(54)-Na(1)-N(51A)-C(514)	-99.3(7)
C(452)-Na(1)-N(51A)-C(514)	68.5(7)
Zn(1)-Na(1)-N(51A)-C(514)	110.8(7)
C(53)-Na(1)-N(51A)-C(514)	-112.6(7)
O(3)-Na(1)-N(51A)-C(52A)	-93.6(6)
N(4)-Na(1)-N(51A)-C(52A)	163.8(4)
N(54A)-Na(1)-N(51A)-C(52A)	25.5(6)
N(51)-Na(1)-N(51A)-C(52A)	76(5)
N(54)-Na(1)-N(51A)-C(52A)	19.3(6)
C(452)-Na(1)-N(51A)-C(52A)	-172.9(6)
Zn(1)-Na(1)-N(51A)-C(52A)	-130.7(4)
C(53)-Na(1)-N(51A)-C(52A)	5.9(4)
O(3)-Na(1)-N(54A)-C(543)	-10.9(6)
N(51A)-Na(1)-N(54A)-C(543)	-118.4(6)
N(4)-Na(1)-N(54A)-C(543)	101.1(5)
N(51)-Na(1)-N(54A)-C(543)	-122.9(6)
N(54)-Na(1)-N(54A)-C(543)	8(3)
C(452)-Na(1)-N(54A)-C(543)	-168.2(4)
Zn(1)-Na(1)-N(54A)-C(543)	42.5(7)
C(53)-Na(1)-N(54A)-C(543)	-82.6(6)
O(3)-Na(1)-N(54A)-C(544)	-125.1(11)
N(51A)-Na(1)-N(54A)-C(544)	127.4(12)
N(4)-Na(1)-N(54A)-C(544)	-13.0(12)
N(51)-Na(1)-N(54A)-C(544)	122.9(12)
N(54)-Na(1)-N(54A)-C(544)	-106(4)
C(452)-Na(1)-N(54A)-C(544)	77.7(13)
Zn(1)-Na(1)-N(54A)-C(544)	-71.7(12)
C(53)-Na(1)-N(54A)-C(544)	163.2(13)
O(3)-Na(1)-N(54A)-C(53A)	104.2(5)
N(51A)-Na(1)-N(54A)-C(53A)	-3.3(6)
N(4)-Na(1)-N(54A)-C(53A)	-143.7(4)
N(51)-Na(1)-N(54A)-C(53A)	-7.8(6)
N(54)-Na(1)-N(54A)-C(53A)	123(4)
C(452)-Na(1)-N(54A)-C(53A)	-53.0(10)
Zn(1)-Na(1)-N(54A)-C(53A)	157.6(4)
C(53)-Na(1)-N(54A)-C(53A)	32.6(3)

C(543)-N(54A)-C(53A)-C(52A)	84.9(14)
C(544)-N(54A)-C(53A)-C(52A)	-161.9(14)
Na(1)-N(54A)-C(53A)-C(52A)	-21.1(7)
N(54A)-C(53A)-C(52A)-N(51A)	50.4(11)
C(513)-N(51A)-C(52A)-C(53A)	-173.1(9)
C(514)-N(51A)-C(52A)-C(53A)	67.6(15)
Na(1)-N(51A)-C(52A)-C(53A)	-49.7(8)

Symmetry transformations used to generate equivalent atoms: