Table 1. Crystal data and structure refinement for cg1.

Identification code	cg1
Empirical formula	$C_{21}H_{31}NNaO_{4.50}$
Formula weight	392.46
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12$
Unit cell dimensions	a = 9.4009(3) Å alpha = 90° b = 14.5547(4) Å beta = 90° c = 16.1500(4) Å gamma = 90°
Volume, Z	2209.76(11) $Å^3$, 4
Density (calculated)	1.180 Mg/m^3
Absorption coefficient	0.098 mm^{-1}
F(000)	844
Crystal size	0.3 x 0.2 x 0.1 mm
θ range for data collection	1.88 to 21.97°
Limiting indices	$-9 \le h \le 7$, $-15 \le k \le 14$, $-16 \le l \le 14$
Reflections collected	8680
Independent reflections	2691 (R_{int} = 0.0620)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2691 / 0 / 259
Goodness-of-fit on F^2	1.065
Final R indices [I>2σ(I)]	R1 = 0.0617, wR2 = 0.1653
R indices (all data)	R1 = 0.0726, wR2 = 0.1754
Absolute structure parameter	-0.9(9)
Extinction coefficient	0.029(6)
Largest diff. peak and hole	0.435 and -0.163 $eÅ^{-3}$

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

	x	y	z	U(eq)
Na(1)	10000	5000	9990(1)	40(1)
Na(2)	9227(4)	5494(2)	8134(2)	43(1)
O(1)	8921(6)	4173(3)	8825(2)	97(2)
O(1X)	10011(11)	5439(5)	7035(5)	80(2)
O(2)	6609(4)	1785(3)	12061(3)	78(1)
O(3)	6977(4)	862(2)	10519(3)	72(1)
O(4)	9090(3)	3810(2)	10702(2)	47(1)
N(1)	7875(4)	1883(2)	9581(3)	54(1)
C(1')	8622(5)	2764(3)	9582(3)	48(1)
C(1)	7632(5)	2268(3)	11821(4)	54(1)
C(2')	8602(5)	3043(3)	10487(3)	41(1)
C(2)	8533(6)	2760(3)	12488(3)	57(1)
C(3')	7937(5)	2350(3)	10953(3)	45(1)
C(3)	8043(6)	3791(4)	12512(3)	67(2)
C(4')	7522(5)	1634(3)	10371(4)	55(1)
C(4)	8500(9)	4264(5)	13289(4)	101(2)
C(5')	8041(6)	1207(4)	8926(4)	70(2)
C(5)	8932(10)	3853(6)	13964(4)	115(3)
C(6')	7945(7)	3430(4)	8985(3)	65(2)
C(6)	9102(7)	2836(6)	14035(4)	91(2)
C(7')	6558(7)	3816(3)	9291(3)	71(2)
C(7)	8699(9)	2487(10)	14898(5)	147(4)
C(8)	8976(10)	1450(8)	14964(6)	163(5)
C(9)	8260(9)	918(7)	14261(7)	168(5)
C(10)	8662(8)	1286(5)	13402(5)	107(3)
C(11)	8290(6)	2337(5)	13354(4)	84(2)
C(12)	10103(5)	2725(3)	12277(3)	56(1)
C(13)	6447(8)	3938(5)	12369(4)	101(2)
C(14)	8518(11)	1081(10)	15840(6)	227(8)

Table 3. Bond lengths [Å] and angles [°] for cq1.

Na(1)-O(4)	2.249(3)	Na(1)-O(4)#1	2.249(3)
Na(1)-O(3)#2	2.388(3)	Na(1)-O(3)#3	2.388(3)
Na(1)-O(1)#1	2.452(4)	Na(1)-O(1)	2.452(4)
Na(1)-Na(2)	3.167(4)	Na(1)-Na(2)#1	3.167(4)
Na(2)-O(1X)	1.924(9)	Na(2)-Na(2)#1	2.044(6)
Na(2)-O(2)#2	2.060(5)	Na(2)-O(1)#1	2.124(6)
Na(2)-O(1)	2.242(5)	Na(2)-O(1X)#1	2.347(8)
Na(2)-O(3)#2	2.511(6)	Na(2)-C(1)#2	3.119(6)
O(1)-C(6')	1.442(6)	O(1)-Na(2)#1	2.124(6)
O(1X)-O(1X)#1	1.277(15)	O(1X)-Na(2)#1	2.347(8)
O(2)-C(1)	1.253(6)	O(2)-Na(2)#4	2.060(5)
O(3)-C(4')	1.258(5)	O(3)-Na(1)#4	2.388(3)
O(3)-Na(2)#4	2.511(6)	O(4)-C(2')	1.256(5)
N(1)-C(4')	1.368(7)	N(1)-C(5')	1.453(6)
N(1)-C(1')	1.462(6)	C(1')-C(6')	1.508(8)
C(1')-C(2')	1.517(6)	C(1)-C(3')	1.435(7)
C(1)-C(2)	1.546(8)	C(1)-Na(2)#4	3.119(6)
C(2')-C(3')	1.405(6)	C(2)-C(12)	1.515(7)
C(2)-C(11)	1.545(7)	C(2)-C(3)	1.570(7)
C(3')-C(4')	1.457(7)	C(3)-C(4)	1.495(9)
C(3)-C(13)	1.533(9)	C(4)-C(5)	1.307(9)
C(5)-C(6)	1.493(11)	C(6')-C(7')	1.503(9)
C(6)-C(11)	1.523(10)	C(6)-C(7)	1.531(9)
C(7)-C(8)	1.536(17)	C(8)-C(9)	1.529(15)
C(8)-C(14)	1.574(11)	C(9)-C(10)	1.535(10)
C(10)-C(11)	1.571(9)		

O(4)-Na(1)-O(4)#1	118.42(17)	O(4)-Na(1)-O(3)#2	106.52(13)
O(4)#1-Na(1)-O(3)#2	93.88(11)	O(4)-Na(1)-O(3)#3	93.88(11)
O(4)#1-Na(1)-O(3)#3	106.52(13)	O(3)#2-Na(1)-O(3)#3	139.8(2)
O(4)-Na(1)-O(1)#1	158.11(14)	O(4)#1-Na(1)-O(1)#1	81.79(11)
O(3)#2-Na(1)-O(1)#1	78.48(17)	O(3)#3-Na(1)-O(1)#1	70.87(16)
O(4)-Na(1)-O(1)	81.79(11)	O(4)#1-Na(1)-O(1)	158.11(14)
O(3)#2-Na(1)-O(1)	70.86(16)	O(3)#3-Na(1)-O(1)	78.48(17)
O(1)#1-Na(1)-O(1)	79.85(17)	O(4)-Na(1)-Na(2)	124.89(11)
O(4)#1-Na(1)-Na(2)	113.38(10)	O(3)#2-Na(1)-Na(2)	51.44(13)
O(3)#3-Na(1)-Na(2)	88.41(14)	O(1)#1-Na(1)-Na(2)	42.06(12)
O(1)-Na(1)-Na(2)	44.83(11)	O(4)-Na(1)-Na(2)#1	113.38(10)
O(4)#1-Na(1)-Na(2)#1	124.89(11)	O(3)#2-Na(1)-Na(2)#1	88.41(14)
O(3)#3-Na(1)-Na(2)#1	51.44(13)	O(1)#1-Na(1)-Na(2)#1	44.83(11)
O(1)-Na(1)-Na(2)#1	42.06(12)	Na(2)-Na(1)-Na(2)#1	37.66(12)
O(1X)-Na(2)-Na(2)#1	72.4(3)	O(1X)-Na(2)-O(2)#2	92.5(3)
Na(2)#1-Na(2)-O(2)#2	155.9(3)	O(1X)-Na(2)-O(1)#1	100.4(4)
Na(2)#1-Na(2)-O(1)#1	65.1(2)	O(2)#2-Na(2)-O(1)#1	100.7(2)
O(1X)-Na(2)-O(1)	118.2(3)	Na(2)#1-Na(2)-O(1)	59.19(19)
O(2)#2-Na(2)-O(1)	144.0(2)	O(1)#1-Na(2)-O(1)	92.2(2)
O(1X)-Na(2)-O(1X)#1	32.9(4)	Na(2)#1-Na(2)-O(1X)#1	51.4(2)
O(2)#2-Na(2)-O(1X)#1	121.9(3)	O(1)#1-Na(2)-O(1X)#1	106.3(3)
O(1)-Na(2)-O(1X)#1	85.4(2)	O(1X)-Na(2)-O(3)#2	168.9(3)

Na(2)#1-Na(2)-O(3)#2	118.07(11)	O(2)#2-Na(2)-O(3)#2	76.45(17)
O(1)#1-Na(2)-O(3)#2	82.25(18)	O(1)-Na(2)-O(3)#2	72.14(17)
O(1X)#1-Na(2)-O(3)#2	156.4(3)	O(1X)-Na(2)-C(1)#2	105.7(3)
Na(2)#1-Na(2)-C(1)#2	168.7(3)	O(2)#2-Na(2)-C(1)#2	15.20(15)
O(1)#1-Na(2)-C(1)#2	104.95(19)	O(1)-Na(2)-C(1)#2	128.8(2)
O(1X)#1-Na(2)-C(1)#2	131.9(3)	O(3)#2-Na(2)-C(1)#2	63.27(14)
O(1X)-Na(2)-Na(1)	140.9(3)	Na(2)#1-Na(2)-Na(1)	71.17(6)
O(2)#2-Na(2)-Na(1)	116.03(17)	O(1)#1-Na(2)-Na(1)	50.67(12)
O(1)-Na(2)-Na(1)	50.45(12)	O(1X)#1-Na(2)-Na(1)	121.0(2)
O(3)#2-Na(2)-Na(1)	48.05(10)	C(1)#2-Na(2)-Na(1)	107.11(14)
C(6')-O(1)-Na(2)#1	141.9(4)	C(6')-O(1)-Na(2)	144.5(4)
Na(2)#1-O(1)-Na(2)	55.76(17)	C(6')-O(1)-Na(1)	119.6(3)
Na(2)#1-O(1)-Na(1)	87.27(17)	Na(2)-O(1)-Na(1)	84.72(14)
O(1X)#1-O(1X)-Na(2)	92.0(5)	O(1X)#1-O(1X)-Na(2)#1	55.0(3)
Na(2)-O(1X)-Na(2)#1	56.2(3)	C(1)-O(2)-Na(2)#4	139.3(4)
C(4')-O(3)-Na(1)#4	136.1(3)	C(4')-O(3)-Na(2)#4	122.6(4)
Na(1)#4-O(3)-Na(2)#4	80.51(14)	C(2')-O(4)-Na(1)	133.0(3)
C(4')-N(1)-C(5')	121.7(4)	C(4')-N(1)-C(1')	110.4(4)
C(5')-N(1)-C(1')	122.9(5)	N(1)-C(1')-C(6')	111.1(4)
N(1)-C(1')-C(2')	103.2(4)	C(6')-C(1')-C(2')	116.0(4)
O(2)-C(1)-C(3')	120.2(5)	O(2)-C(1)-C(2)	117.7(5)
C(3')-C(1)-C(2)	122.1(4)	O(2)-C(1)-Na(2)#4	25.5(3)
C(3')-C(1)-Na(2)#4	101.8(3)	C(2)-C(1)-Na(2)#4	132.4(3)
O(4)-C(2')-C(3')	130.7(4)	O(4)-C(2')-C(1')	120.0(4)
C(3')-C(2')-C(1')	109.3(4)	C(12)-C(2)-C(1)	111.2(4)
C(12)-C(2)-C(11)	109.5(4)	C(1)-C(2)-C(11)	111.4(5)
C(12)-C(2)-C(3)	108.9(4)	C(1)-C(2)-C(3)	107.4(4)
C(11)-C(2)-C(3)	108.4(5)	C(2')-C(3')-C(1)	132.2(4)
C(2')-C(3')-C(4')	106.7(4)	C(1)-C(3')-C(4')	121.1(4)
C(4)-C(3)-C(13)	110.1(5)	C(4)-C(3)-C(2)	112.1(5)
C(13)-C(3)-C(2)	114.6(6)	O(3)-C(4')-N(1)	120.9(5)
O(3)-C(4')-C(3')	128.8(6)	N(1)-C(4')-C(3')	110.3(4)
C(5)-C(4)-C(3)	125.3(7)	C(4)-C(5)-C(6)	123.4(7)
O(1)-C(6')-C(7')	109.3(5)	O(1)-C(6')-C(1')	109.1(5)
C(7')-C(6')-C(1')	113.3(4)	C(5)-C(6)-C(11)	111.3(6)
C(5)-C(6)-C(7)	111.9(8)	C(11)-C(6)-C(7)	112.0(7)
C(6)-C(7)-C(8)	110.3(9)	C(9)-C(8)-C(7)	111.8(7)
C(9)-C(8)-C(14)	112.0(8)	C(7)-C(8)-C(14)	110.6(11)
C(8)-C(9)-C(10)	112.7(7)	C(9)-C(10)-C(11)	109.2(7)
C(6)-C(11)-C(2)	112.9(5)	C(6)-C(11)-C(10)	108.5(5)
C(2)-C(11)-C(10)	113.5(6)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,z #2 -x+3/2,y+1/2,-z+2 #3 x+1/2,-y+1/2,-z+2

#4 -x+3/2,y-1/2,-z+2

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for cq1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Na(1)	43(1)	19(1)	57(1)	0	0	-3(1)
Na(2)	40(2)	29(2)	61(2)	-3(2)	-9(2)	9(2)
O(1)	149(4)	83(3)	59(2)	-3(2)	11(2)	-92(3)
O(1X)	106(6)	67(4)	68(4)	5(3)	0(5)	21(5)
O(2)	43(2)	67(2)	123(3)	46(2)	10(2)	-3(2)
O(3)	51(2)	23(2)	142(3)	18(2)	-30(2)	-10(2)
O(4)	55(2)	26(2)	60(2)	-5(1)	6(2)	-10(2)
N(1)	47(2)	26(2)	88(3)	-13(2)	1(2)	-6(2)
C(1')	34(2)	38(3)	73(3)	-11(2)	10(2)	-16(2)
C(1)	36(3)	37(3)	89(4)	24(3)	6(3)	3(2)
C(2')	35(2)	27(3)	61(3)	-4(2)	2(2)	1(2)
C(2)	53(3)	49(3)	68(3)	17(3)	13(3)	8(3)
C(3')	35(2)	23(2)	79(3)	10(2)	-1(2)	-4(2)
C(3)	75(4)	67(3)	59(3)	12(3)	16(3)	27(3)
C(4')	29(3)	22(3)	115(5)	3(3)	-10(3)	4(2)
C(4)	138(7)	93(5)	71(4)	-6(4)	7(4)	51(5)
C(5')	46(3)	43(3)	122(5)	-37(3)	-8(3)	0(2)
C(5)	153(8)	130(7)	61(4)	8(4)	13(4)	48(6)
C(6')	84(4)	48(3)	63(3)	-2(3)	0(3)	-42(3)
C(6)	64(4)	143(7)	67(4)	46(4)	10(3)	10(4)
C(7')	94(5)	33(3)	85(4)	6(3)	-26(4)	-5(3)
C(7)	80(5)	275(13)	85(5)	84(7)	8(4)	-1(7)
C(8)	89(6)	243(13)	157(8)	142(9)	-39(7)	-37(8)
C(9)	79(5)	186(10)	238(11)	179(10)	-43(7)	-39(6)
C(10)	76(4)	91(5)	153(7)	79(5)	-23(5)	-6(4)
C(11)	51(3)	112(5)	89(4)	65(4)	13(3)	10(4)
C(12)	48(3)	46(3)	76(3)	0(3)	5(3)	1(3)
C(13)	90(5)	112(6)	101(5)	15(4)	10(4)	54(5)
C(14)	93(6)	410(20)	184(10)	210(13)	-20(7)	-55(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for cq1.

	x	y	z	U(eq)
H(1'A)	9631	2659	9409	58
H(3A)	8544	4108	12046	80
H(4A)	8475	4917	13293	121
H(5'A)	7430	676	9041	105
H(5'B)	9035	1007	8901	105
H(5'C)	7768	1481	8395	105
H(5A)	9149	4221	14433	138
H(6'A)	7763	3100	8452	78
H(6A)	10134	2697	13952	110
H(7'A)	6171	4240	8877	106
H(7'B)	6718	4147	9811	106
H(7'C)	5882	3314	9384	106
H(7A)	7680	2614	15004	176
H(7B)	9266	2815	15321	176
H(8A)	10025	1353	14910	196
H(9A)	7215	955	14330	201
H(9B)	8537	263	14299	201
H(10A)	8132	946	12970	128
H(10B)	9693	1196	13304	128
H(11A)	7254	2399	13482	100
H(12A)	10418	2084	12259	85
H(12B)	10644	3057	12701	85
H(12C)	10261	3012	11736	85
H(13A)	6230	4596	12396	152
H(13B)	5907	3612	12797	152
H(13C)	6184	3700	11822	152
H(14A)	8997	1438	16272	341
H(14B)	8787	433	15891	341
H(14C)	7486	1142	15903	341