

C(12)	12098(5)	1791(4)	4153(5)	77(3)	
C(13)	10812(6)	2428(3)	3721(5)	66(2)	
C(14)	10579(5)	1736(3)	4835(4)	55(2)	
C(15)	11067(4)	1249(2)	2594(4)	31(1)	
C(30)	12072(4)	376(2)	1800(4)	25(1)	
C(31)	11919(4)	-143(2)	1929(4)	28(1)	
C(32)	12631(4)	-415(2)	2544(4)	33(1)	
C(33)	12524(4)	-981(2)	2697(4)	40(2)	
C(34)	13353(5)	-1198(3)	3395(5)	63(2)	
C(35)	12533(5)	-1257(2)	1764(5)	54(2)	
C(36)	11591(5)	-1087(2)	3093(4)	50(2)	
C(37)	13426(4)	-160(2)	2990(4)	38(2)	
C(38)	13603(4)	343(2)	2858(4)	35(1)	
C(39)	14488(4)	598(2)	3410(5)	48(2)	
C(40)	14614(5)	1134(3)	3076(6)	75(3)	
C(41)	14352(5)	616(3)	4457(5)	64(2)	
C(42)	15401(5)	303(3)	3295(5)	63(2)	
C(43)	12918(4)	595(2)	2241(4)	31(1)	
C(16)	11738(4)	1040(2)	510(3)	25(1)	
C(17)	11706(4)	905(2)	-458(4)	27(1)	
C(18)	12170(4)	1227(2)	-1051(4)	32(1)	
C(19)	12127(5)	1117(2)	-2116(4)	44(2)	
C(20)	12670(6)	1511(3)	-2624(5)	69(2)	
C(21)	12570(6)	602(3)	-2277(5)	58(2)	
C(22)	11070(5)	1133(3)	-2587(4)	55(2)	
C(23)	12641(4)	1648(2)	-662(4)	36(1)	
C(24)	12663(4)	1793(2)	279(4)	33(1)	
C(25)	13215(5)	2258(2)	662(4)	39(2)	
C(26)	14298(5)	2161(3)	725(5)	55(2)	
C(27)	12997(6)	2388(2)	1655(4)	54(2)	
C(28)	12935(5)	2708(2)	21(5)	52(2)	
C(29)	12186(4)	1484(2)	831(4)	27(1)	
O(101)	9765(4)	1884(2)	-445(4)	70(2)	
C(101)	10113(6)	2173(3)	399(6)	70(2)	
C(102)	9534(7)	2615(4)	610(8)	104(3)	
C(103)	9604(6)	2187(3)	-1247(6)	82(3)	
C(104)	10444(7)	2459(3)	-1503(6)	82(3)	
O(301)	10916(11)	151(6)	4467(11)	172(6)	0.666
C(301)	9825(11)	179(6)	4252(10)	102(5)	0.666
C(302)	9584(8)	139(4)	3446(7)	52(3)	0.666
C(303)	10878(8)	-284(5)	5165(12)	96(5)	0.666
C(304)	11883(13)	-343(9)	5483(17)	177(9)	0.666
O(201)	14300(11)	479(6)	158(11)	176(6)	0.666
C(201)	14330(12)	-82(6)	266(14)	122(6)	0.666
C(202)	13485(8)	-247(5)	256(8)	71(4)	0.666
C(203)	14972(13)	428(7)	-612(12)	120(6)	0.666
C(204)	15100(20)	974(9)	-660(20)	224(12)	0.666

Table 22. Bond lengths [Å] and angles [deg] for 3a·4²-Et₂O.

Na(1)-O(1)	2.299(4)	C(9)-C(10)	1.398(8)
Na(1)-O(3)#1	2.333(4)	C(10)-C(15)	1.384(8)
Na(1)-O(101)	2.447(5)	C(10)-C(11)	1.526(8)
Na(1)-O(2)	2.451(4)	C(11)-C(13)	1.526(10)
Na(1)-C(17)	2.691(6)	C(11)-C(14)	1.530(9)
Na(1)-C(16)	2.966(5)	C(11)-C(12)	1.541(9)
Na(1)-C(3)	3.043(5)	C(30)-C(43)	1.393(7)
Na(1)-Na(2)#1	3.161(3)	C(30)-C(31)	1.422(8)
Na(1)-Na(3)#1	3.237(3)	C(31)-C(32)	1.435(8)
Na(1)-Na(3)	4.214(3)	C(32)-C(37)	1.386(8)

Na(1)-Na(2)	4.217(3)	C(32)-C(33)	1.542(8)
Na(3)-O(2)#1	2.234(4)	C(33)-C(36)	1.523(9)
Na(3)-O(3)	2.281(4)	C(33)-C(35)	1.528(9)
Na(3)-O(1)	2.392(4)	C(33)-C(34)	1.538(8)
Na(3)-C(3)	2.668(6)	C(37)-C(38)	1.388(8)
Na(3)-C(2)	2.920(6)	C(38)-C(43)	1.387(8)
Na(3)-C(1)	3.057(6)	C(38)-C(39)	1.535(8)
Na(3)-C(31)	3.068(6)	C(39)-C(40)	1.531(9)
Na(3)-Na(2)#1	3.119(3)	C(39)-C(42)	1.532(10)
Na(3)-Na(1)#1	3.237(3)	C(39)-C(41)	1.538(10)
Na(3)-Na(2)	4.038(3)	C(16)-C(29)	1.393(7)
Na(2)-O(1)#1	2.234(4)	C(16)-C(17)	1.426(7)
Na(2)-O(2)	2.290(4)	C(17)-C(18)	1.428(8)
Na(2)-O(3)	2.376(4)	C(18)-C(23)	1.386(8)
Na(2)-C(31)	2.681(5)	C(18)-C(19)	1.545(8)
Na(2)-C(30)	2.932(5)	C(19)-C(22)	1.542(9)
Na(2)-C(1)	3.038(6)	C(19)-C(20)	1.542(9)
Na(2)-C(17)	3.050(6)	C(19)-C(21)	1.545(9)
Na(2)-Na(3)#1	3.119(3)	C(23)-C(24)	1.399(8)
Na(2)-Na(1)#1	3.161(3)	C(24)-C(29)	1.380(7)
O(1)-C(3)	1.325(6)	C(24)-C(25)	1.527(8)
O(1)-Na(2)#1	2.234(4)	C(25)-C(26)	1.531(9)
C(1)-C(16)	1.536(7)	C(25)-C(28)	1.532(8)
C(1)-C(2)	1.544(7)	C(25)-C(27)	1.536(8)
C(1)-C(30)	1.547(7)	O(101)-C(103)	1.398(9)
C(2)-C(15)	1.389(7)	O(101)-C(101)	1.460(9)
C(2)-C(3)	1.417(7)	C(101)-C(102)	1.491(12)
C(3)-C(4)	1.441(8)	C(103)-C(104)	1.474(11)
O(3)-C(31)	1.349(6)	O(301)-C(301)	1.519(15)
O(3)-Na(1)#1	2.333(4)	O(301)-C(303)	1.541(15)
O(2)-C(17)	1.331(6)	C(301)-C(302)	1.162(13)
O(2)-Na(3)#1	2.234(4)	C(303)-C(304)	1.428(16)
C(4)-C(9)	1.389(8)	O(201)-C(201)	1.509(15)
C(4)-C(5)	1.529(8)	O(201)-C(203)	1.552(15)
C(5)-C(7)	1.527(9)	C(201)-C(202)	1.263(14)
C(5)-C(8)	1.534(9)	C(203)-C(204)	1.475(18)
C(5)-C(6)	1.540(9)		

O(1)-Na(1)-O(3)#1	93.01(14)	O(2)-Na(2)-Na(1)	28.23(10)
O(1)-Na(1)-O(101)	102.51(18)	O(3)-Na(2)-Na(1)	89.97(11)
O(3)#1-Na(1)-O(101)	136.69(17)	C(31)-Na(2)-Na(1)	97.12(13)
O(1)-Na(1)-O(2)	109.18(14)	C(30)-Na(2)-Na(1)	78.38(12)
O(3)#1-Na(1)-O(2)	88.14(14)	C(1)-Na(2)-Na(1)	48.42(10)
O(101)-Na(1)-O(2)	122.79(17)	C(17)-Na(2)-Na(1)	39.52(10)
O(1)-Na(1)-C(17)	111.72(16)	Na(3)#1-Na(2)-Na(1)	49.65(6)
O(3)#1-Na(1)-C(17)	116.86(17)	Na(1)#1-Na(2)-Na(1)	94.73(7)
O(101)-Na(1)-C(17)	94.60(18)	Na(3)-Na(2)-Na(1)	61.34(5)
O(2)-Na(1)-C(17)	29.53(14)	C(3)-O(1)-Na(2)#1	159.5(3)
O(1)-Na(1)-C(16)	87.46(14)	C(3)-O(1)-Na(1)	111.4(3)
O(3)#1-Na(1)-C(16)	136.23(16)	Na(2)#1-O(1)-Na(1)	88.42(14)
O(101)-Na(1)-C(16)	85.22(16)	C(3)-O(1)-Na(3)	86.7(3)
O(2)-Na(1)-C(16)	51.12(13)	Na(2)#1-O(1)-Na(3)	84.72(14)
C(17)-Na(1)-C(16)	28.68(15)	Na(1)-O(1)-Na(3)	127.86(17)
O(1)-Na(1)-C(3)	23.90(13)	C(16)-C(1)-C(2)	112.2(4)
O(3)#1-Na(1)-C(3)	116.90(15)	C(16)-C(1)-C(30)	112.2(4)
O(101)-Na(1)-C(3)	84.50(17)	C(2)-C(1)-C(30)	112.2(4)
O(2)-Na(1)-C(3)	107.31(14)	C(16)-C(1)-Na(2)	89.5(3)
C(17)-Na(1)-C(3)	98.03(16)	C(2)-C(1)-Na(2)	152.7(3)
C(16)-Na(1)-C(3)	70.18(15)	C(30)-C(1)-Na(2)	71.2(3)
O(1)-Na(1)-Na(2)#1	44.95(10)	C(16)-C(1)-Na(3)	153.2(3)
O(3)#1-Na(1)-Na(2)#1	48.41(10)	C(2)-C(1)-Na(3)	70.2(3)
O(101)-Na(1)-Na(2)#1	128.42(16)	C(30)-C(1)-Na(3)	89.7(3)
O(2)-Na(1)-Na(2)#1	107.33(12)	Na(2)-C(1)-Na(3)	83.00(14)

C(17)-Na(1)-Na(2)#1	131.11(14)	C(15)-C(2)-C(3)	119.9(5)
C(16)-Na(1)-Na(2)#1	122.02(13)	C(15)-C(2)-C(1)	120.5(5)
C(3)-Na(1)-Na(2)#1	68.78(11)	C(3)-C(2)-C(1)	119.5(4)
O(1)-Na(1)-Na(3)#1	109.11(12)	C(15)-C(2)-Na(3)	128.0(4)
O(3)#1-Na(1)-Na(3)#1	44.79(11)	C(3)-C(2)-Na(3)	65.6(3)
O(101)-Na(1)-Na(3)#1	148.31(16)	C(1)-C(2)-Na(3)	80.0(3)
O(2)-Na(1)-Na(3)#1	43.59(9)	O(1)-C(3)-C(2)	120.1(5)
C(17)-Na(1)-Na(3)#1	72.09(13)	O(1)-C(3)-C(4)	121.7(5)
C(16)-Na(1)-Na(3)#1	94.04(12)	C(2)-C(3)-C(4)	118.1(5)
C(3)-Na(1)-Na(3)#1	125.04(13)	O(1)-C(3)-Na(3)	63.6(3)
Na(2)#1-Na(1)-Na(3)#1	78.27(7)	C(2)-C(3)-Na(3)	85.5(3)
O(1)-Na(1)-Na(3)	26.63(10)	C(4)-C(3)-Na(3)	121.5(4)
O(3)#1-Na(1)-Na(3)	86.27(11)	O(1)-C(3)-Na(1)	44.7(2)
O(101)-Na(1)-Na(3)	123.56(15)	C(2)-C(3)-Na(1)	94.5(3)
O(2)-Na(1)-Na(3)	83.23(10)	C(4)-C(3)-Na(1)	131.0(4)
C(17)-Na(1)-Na(3)	92.09(13)	Na(3)-C(3)-Na(1)	94.87(17)
C(16)-Na(1)-Na(3)	74.99(11)	C(31)-O(3)-Na(3)	112.9(3)
C(3)-Na(1)-Na(3)	39.11(11)	C(31)-O(3)-Na(1)#1	157.7(3)
Na(2)#1-Na(1)-Na(3)	47.44(5)	Na(3)-O(3)-Na(1)#1	89.09(14)
Na(3)#1-Na(1)-Na(3)	86.36(7)	C(31)-O(3)-Na(2)	87.5(3)
O(1)-Na(1)-Na(2)	83.60(11)	Na(3)-O(3)-Na(2)	120.27(17)
O(3)#1-Na(1)-Na(2)	83.56(11)	Na(1)#1-O(3)-Na(2)	84.32(14)
O(101)-Na(1)-Na(2)	137.72(14)	C(17)-O(2)-Na(3)#1	160.2(3)
O(2)-Na(1)-Na(2)	26.23(9)	C(17)-O(2)-Na(2)	112.0(3)
C(17)-Na(1)-Na(2)	46.16(12)	Na(3)#1-O(2)-Na(2)	87.16(14)
C(16)-Na(1)-Na(2)	52.96(11)	C(17)-O(2)-Na(1)	85.3(3)
C(3)-Na(1)-Na(2)	86.37(11)	Na(3)#1-O(2)-Na(1)	87.26(14)
Na(2)#1-Na(1)-Na(2)	85.27(7)	Na(2)-O(2)-Na(1)	125.53(17)
Na(3)#1-Na(1)-Na(2)	47.26(6)	C(9)-C(4)-C(3)	117.9(5)
Na(3)-Na(1)-Na(2)	57.24(5)	C(9)-C(4)-C(5)	120.9(5)
O(2)#1-Na(3)-O(3)	94.99(15)	C(3)-C(4)-C(5)	121.2(5)
O(2)#1-Na(3)-O(1)	92.51(14)	C(7)-C(5)-C(4)	109.7(5)
O(3)-Na(3)-O(1)	115.88(16)	C(7)-C(5)-C(8)	109.5(5)
O(2)#1-Na(3)-C(3)	121.17(17)	C(4)-C(5)-C(8)	111.3(5)
O(3)-Na(3)-C(3)	116.03(17)	C(7)-C(5)-C(6)	106.8(6)
O(1)-Na(3)-C(3)	29.72(13)	C(4)-C(5)-C(6)	112.6(5)
O(2)#1-Na(3)-C(2)	141.99(16)	C(8)-C(5)-C(6)	106.8(6)
O(3)-Na(3)-C(2)	90.40(15)	C(4)-C(9)-C(10)	124.8(5)
O(1)-Na(3)-C(2)	52.00(13)	C(15)-C(10)-C(9)	115.6(5)
C(3)-Na(3)-C(2)	28.94(15)	C(15)-C(10)-C(11)	123.9(5)
O(2)#1-Na(3)-C(1)	126.89(16)	C(9)-C(10)-C(11)	120.5(5)
O(3)-Na(3)-C(1)	63.45(14)	C(13)-C(11)-C(10)	109.7(5)
O(1)-Na(3)-C(1)	61.74(13)	C(13)-C(11)-C(14)	109.5(6)
C(3)-Na(3)-C(1)	52.59(15)	C(10)-C(11)-C(14)	110.2(5)
C(2)-Na(3)-C(1)	29.84(14)	C(13)-C(11)-C(12)	108.9(6)
O(2)#1-Na(3)-C(31)	118.87(16)	C(10)-C(11)-C(12)	111.5(5)
O(3)-Na(3)-C(31)	23.89(13)	C(14)-C(11)-C(12)	107.0(6)
O(1)-Na(3)-C(31)	110.77(15)	C(10)-C(15)-C(2)	123.6(5)
C(3)-Na(3)-C(31)	99.59(17)	C(43)-C(30)-C(31)	119.1(5)
C(2)-Na(3)-C(31)	71.24(15)	C(43)-C(30)-C(1)	120.4(5)
C(1)-Na(3)-C(31)	49.79(14)	C(31)-C(30)-C(1)	120.5(4)
O(2)#1-Na(3)-Na(2)#1	47.17(11)	C(43)-C(30)-Na(2)	128.6(4)
O(3)-Na(3)-Na(2)#1	115.32(13)	C(31)-C(30)-Na(2)	65.7(3)
O(1)-Na(3)-Na(2)#1	45.49(10)	C(1)-C(30)-Na(2)	78.8(3)
C(3)-Na(3)-Na(2)#1	74.11(13)	O(3)-C(31)-C(30)	119.8(5)
C(2)-Na(3)-Na(2)#1	96.93(12)	O(3)-C(31)-C(32)	122.0(5)
C(1)-Na(3)-Na(2)#1	96.59(12)	C(30)-C(31)-C(32)	118.2(5)
C(31)-Na(3)-Na(2)#1	130.10(13)	O(3)-C(31)-Na(2)	62.3(2)
O(2)#1-Na(3)-Na(1)#1	49.15(11)	C(30)-C(31)-Na(2)	85.4(3)
O(3)-Na(3)-Na(1)#1	46.12(10)	C(32)-C(31)-Na(2)	122.5(4)
O(1)-Na(3)-Na(1)#1	115.25(12)	O(3)-C(31)-Na(3)	43.2(2)
C(3)-Na(3)-Na(1)#1	139.06(15)	C(30)-C(31)-Na(3)	91.6(3)
C(2)-Na(3)-Na(1)#1	128.09(13)	C(32)-C(31)-Na(3)	136.1(4)

C(1)-Na(3)-Na(1)#1	98.32(12)	Na(2)-C(31)-Na(3)	88.98(16)
C(31)-Na(3)-Na(1)#1	69.96(12)	C(37)-C(32)-C(31)	118.5(5)
Na(2)#1-Na(3)-Na(1)#1	83.10(8)	C(37)-C(32)-C(33)	120.6(5)
O(2)#1-Na(3)-Na(2)	87.82(12)	C(31)-C(32)-C(33)	121.0(5)
O(3)-Na(3)-Na(2)	30.53(10)	C(36)-C(33)-C(35)	110.4(5)
O(1)-Na(3)-Na(2)	86.65(11)	C(36)-C(33)-C(34)	107.3(5)
C(3)-Na(3)-Na(2)	95.30(13)	C(35)-C(33)-C(34)	106.7(5)
C(2)-Na(3)-Na(2)	78.06(12)	C(36)-C(33)-C(32)	110.0(5)
C(1)-Na(3)-Na(2)	48.30(11)	C(35)-C(33)-C(32)	109.8(5)
C(31)-Na(3)-Na(2)	41.59(10)	C(34)-C(33)-C(32)	112.6(5)
Na(2)#1-Na(3)-Na(2)	88.95(8)	C(32)-C(37)-C(38)	124.4(5)
Na(1)#1-Na(3)-Na(2)	50.03(6)	C(43)-C(38)-C(37)	115.9(5)
O(2)#1-Na(3)-Na(1)	87.86(11)	C(43)-C(38)-C(39)	123.4(5)
O(3)-Na(3)-Na(1)	91.35(12)	C(37)-C(38)-C(39)	120.6(5)
O(1)-Na(3)-Na(1)	25.51(9)	C(40)-C(39)-C(42)	108.4(6)
C(3)-Na(3)-Na(1)	46.03(12)	C(40)-C(39)-C(38)	112.1(5)
C(2)-Na(3)-Na(1)	54.35(11)	C(42)-C(39)-C(38)	110.0(6)
C(1)-Na(3)-Na(1)	48.43(10)	C(40)-C(39)-C(41)	108.2(6)
C(31)-Na(3)-Na(1)	91.33(11)	C(42)-C(39)-C(41)	109.9(5)
Na(2)#1-Na(3)-Na(1)	48.28(6)	C(38)-C(39)-C(41)	108.3(5)
Na(1)#1-Na(3)-Na(1)	93.64(7)	C(38)-C(43)-C(30)	123.7(5)
Na(2)-Na(3)-Na(1)	61.41(5)	C(29)-C(16)-C(17)	119.2(5)
O(1)#1-Na(2)-O(2)	95.31(15)	C(29)-C(16)-C(1)	120.2(4)
O(1)#1-Na(2)-O(3)	93.54(14)	C(17)-C(16)-C(1)	120.6(5)
O(2)-Na(2)-O(3)	117.21(16)	C(29)-C(16)-Na(1)	124.5(3)
O(1)#1-Na(2)-C(31)	122.63(17)	C(17)-C(16)-Na(1)	64.9(3)
O(2)-Na(2)-C(31)	116.54(17)	C(1)-C(16)-Na(1)	82.7(3)
O(3)-Na(2)-C(31)	30.17(14)	O(2)-C(17)-C(16)	119.6(5)
O(1)#1-Na(2)-C(30)	143.44(16)	O(2)-C(17)-C(18)	122.3(5)
O(2)-Na(2)-C(30)	90.57(15)	C(16)-C(17)-C(18)	118.1(5)
O(3)-Na(2)-C(30)	52.42(14)	O(2)-C(17)-Na(1)	65.2(3)
C(31)-Na(2)-C(30)	28.90(16)	C(16)-C(17)-Na(1)	86.4(3)
O(1)#1-Na(2)-C(1)	128.50(16)	C(18)-C(17)-Na(1)	117.4(4)
O(2)-Na(2)-C(1)	63.39(14)	O(2)-C(17)-Na(2)	44.1(2)
O(3)-Na(2)-C(1)	62.96(14)	C(16)-C(17)-Na(2)	91.1(3)
C(31)-Na(2)-C(1)	53.15(15)	C(18)-C(17)-Na(2)	136.5(4)
C(30)-Na(2)-C(1)	29.97(14)	Na(1)-C(17)-Na(2)	94.32(17)
O(1)#1-Na(2)-C(17)	119.17(15)	C(23)-C(18)-C(17)	118.9(5)
O(2)-Na(2)-C(17)	23.86(13)	C(23)-C(18)-C(19)	120.1(5)
O(3)-Na(2)-C(17)	112.31(15)	C(17)-C(18)-C(19)	121.0(5)
C(31)-Na(2)-C(17)	100.12(16)	C(22)-C(19)-C(20)	106.4(5)
C(30)-Na(2)-C(17)	71.64(15)	C(22)-C(19)-C(21)	110.0(5)
C(1)-Na(2)-C(17)	50.00(14)	C(20)-C(19)-C(21)	107.8(6)
O(1)#1-Na(2)-Na(3)#1	49.79(11)	C(22)-C(19)-C(18)	109.2(5)
O(2)-Na(2)-Na(3)#1	45.68(10)	C(20)-C(19)-C(18)	112.5(5)
O(3)-Na(2)-Na(3)#1	116.22(12)	C(21)-C(19)-C(18)	110.9(5)
C(31)-Na(2)-Na(3)#1	139.89(15)	C(18)-C(23)-C(24)	123.9(5)
C(30)-Na(2)-Na(3)#1	127.95(13)	C(29)-C(24)-C(23)	116.0(5)
C(1)-Na(2)-Na(3)#1	98.05(12)	C(29)-C(24)-C(25)	123.1(5)
C(17)-Na(2)-Na(3)#1	69.47(11)	C(23)-C(24)-C(25)	120.9(5)
O(1)#1-Na(2)-Na(1)#1	46.63(10)	C(24)-C(25)-C(26)	109.3(5)
O(2)-Na(2)-Na(1)#1	118.06(12)	C(24)-C(25)-C(28)	110.6(5)
O(3)-Na(2)-Na(1)#1	47.27(10)	C(26)-C(25)-C(28)	109.8(5)
C(31)-Na(2)-Na(1)#1	76.02(13)	C(24)-C(25)-C(27)	111.1(5)
C(30)-Na(2)-Na(1)#1	99.35(13)	C(26)-C(25)-C(27)	107.9(5)
C(1)-Na(2)-Na(1)#1	100.39(12)	C(28)-C(25)-C(27)	108.1(5)
C(17)-Na(2)-Na(1)#1	133.95(13)	C(24)-C(29)-C(16)	123.7(5)
Na(3)#1-Na(2)-Na(1)#1	84.28(8)	C(103)-O(101)-C(101)	111.7(6)
O(1)#1-Na(2)-Na(3)	87.89(11)	C(103)-O(101)-Na(1)	121.3(5)
O(2)-Na(2)-Na(3)	89.31(11)	C(101)-O(101)-Na(1)	125.8(4)
O(3)-Na(2)-Na(3)	29.19(10)	O(101)-C(101)-C(102)	117.4(7)
C(31)-Na(2)-Na(3)	49.43(12)	O(101)-C(103)-C(104)	116.5(7)
C(30)-Na(2)-Na(3)	56.06(11)	C(301)-O(301)-C(303)	92.5(11)

C(1)-Na(2)-Na(3)	48.70(10)	C(302)-C(301)-O(301)	109.9(15)
C(17)-Na(2)-Na(3)	90.49(12)	C(304)-C(303)-O(301)	99.7(14)
Na(3)#1-Na(2)-Na(3)	91.05(8)	C(201)-O(201)-C(203)	88.6(12)
Na(1)#1-Na(2)-Na(3)	51.70(6)	C(202)-C(201)-O(201)	109.5(16)
O(1)#1-Na(2)-Na(1)	90.11(11)	C(204)-C(203)-O(201)	92.1(16)

Symmetry transformations used to generate equivalent atoms:
 #1 -x+2,-y,-z

Table 23. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $3a \cdot 4\frac{1}{2}\text{Et}_2\text{O}$.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Na(1)	35(1)	34(1)	34(1)	3(1)	1(1)	-2(1)
Na(3)	38(1)	31(1)	47(1)	-2(1)	-2(1)	-3(1)
Na(2)	43(1)	33(1)	31(1)	-1(1)	-1(1)	-5(1)
O(1)	26(2)	32(2)	25(2)	-6(2)	1(2)	-1(2)
C(1)	24(3)	23(3)	20(3)	1(2)	2(2)	-4(2)
C(2)	26(3)	25(3)	22(3)	0(2)	2(2)	0(2)
C(3)	31(3)	26(3)	20(3)	2(2)	-2(2)	-3(2)
O(3)	31(2)	29(2)	29(2)	2(2)	-4(2)	-5(2)
O(2)	36(2)	29(2)	24(2)	-3(2)	2(2)	-10(2)
C(4)	30(3)	34(3)	34(3)	-3(3)	7(3)	2(3)
C(5)	32(4)	52(4)	45(4)	-19(3)	4(3)	-1(3)
C(6)	31(4)	87(6)	89(6)	-37(5)	12(4)	11(4)
C(7)	35(4)	71(5)	55(4)	-9(4)	13(3)	-6(3)
C(8)	42(4)	67(5)	57(4)	-5(4)	-6(3)	15(4)
C(9)	39(4)	43(4)	33(3)	-15(3)	9(3)	-1(3)
C(10)	38(4)	40(4)	28(3)	-9(3)	7(3)	-2(3)
C(11)	39(4)	65(5)	35(4)	-19(3)	6(3)	-5(3)
C(12)	42(4)	131(8)	57(5)	-56(5)	4(4)	-17(5)
C(13)	85(6)	60(5)	53(4)	-25(4)	9(4)	-21(4)
C(14)	62(5)	66(5)	36(4)	-19(3)	2(3)	5(4)
C(15)	33(3)	34(3)	25(3)	-2(3)	4(3)	-3(3)
C(30)	26(3)	27(3)	24(3)	-1(2)	5(2)	-2(2)
C(31)	29(3)	29(3)	24(3)	0(3)	1(2)	-2(3)
C(32)	37(3)	31(3)	29(3)	4(3)	0(3)	4(3)
C(33)	40(4)	30(3)	45(4)	6(3)	-7(3)	2(3)
C(34)	62(5)	40(4)	76(5)	21(4)	-25(4)	0(4)
C(35)	64(5)	34(4)	60(4)	-2(3)	0(4)	11(3)
C(36)	67(5)	36(4)	43(4)	10(3)	0(3)	-4(3)
C(37)	36(3)	34(4)	40(3)	10(3)	-11(3)	1(3)
C(38)	33(3)	33(4)	34(3)	3(3)	-7(3)	-4(3)
C(39)	35(4)	44(4)	59(4)	12(3)	-17(3)	-9(3)
C(40)	54(5)	57(5)	101(6)	9(4)	-36(4)	-25(4)
C(41)	59(5)	70(5)	57(5)	-15(4)	-22(4)	-7(4)
C(42)	36(4)	72(5)	75(5)	14(4)	-15(4)	-4(4)
C(43)	33(3)	30(3)	32(3)	6(3)	5(3)	-4(3)
C(16)	21(3)	26(3)	27(3)	1(2)	0(2)	3(2)
C(17)	26(3)	30(3)	25(3)	1(3)	4(2)	1(3)
C(18)	37(3)	36(3)	22(3)	0(3)	4(3)	-6(3)
C(19)	58(4)	46(4)	28(3)	0(3)	11(3)	-16(3)
C(20)	95(6)	84(6)	32(4)	-1(4)	21(4)	-36(5)
C(21)	76(5)	64(5)	38(4)	-15(3)	21(4)	-8(4)
C(22)	75(5)	58(5)	29(3)	7(3)	-4(3)	-13(4)

C(23)	45(4)	32(3)	31(3)	6(3)	7(3)	-11(3)
C(24)	44(4)	30(3)	23(3)	4(3)	2(3)	-4(3)
C(25)	54(4)	28(3)	33(3)	2(3)	-2(3)	-11(3)
C(26)	59(5)	47(4)	57(4)	7(3)	-5(4)	-25(4)
C(27)	86(5)	34(4)	41(4)	-10(3)	4(4)	-27(4)
C(28)	74(5)	28(4)	52(4)	5(3)	4(4)	-19(3)
C(29)	29(3)	26(3)	24(3)	-3(2)	2(2)	-1(3)
O(101)	72(4)	53(3)	77(4)	19(3)	-22(3)	-15(3)
C(101)	75(6)	57(5)	74(5)	7(4)	-4(4)	-3(4)
C(102)	96(7)	72(7)	139(9)	-12(6)	-2(7)	9(6)
C(103)	82(6)	60(5)	96(7)	24(5)	-13(5)	-7(5)
C(104)	98(7)	63(6)	79(6)	19(5)	-9(5)	-13(5)
C(302)	67(7)	45(6)	51(6)	21(5)	30(5)	19(5)
C(303)	38(7)	97(11)	156(14)	-32(10)	26(8)	-1(7)
C(202)	58(7)	110(10)	50(7)	8(7)	26(6)	33(7)

Table 24. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**·4Et₂O.

	x	y	z	U(eq)
H(1A)	10876	462	807	27
H(6A)	7692	1576	3127	103
H(6B)	6830	1670	2324	103
H(6C)	7743	2013	2409	103
H(7A)	7704	702	2589	80
H(7B)	7819	575	1542	80
H(7C)	6866	821	1775	80
H(8A)	7955	1299	387	85
H(8B)	7895	1847	762	85
H(8C)	6986	1500	674	85
H(9A)	9187	1776	3155	46
H(12A)	12357	1984	4695	115
H(12B)	12396	1893	3619	115
H(12C)	12225	1443	4277	115
H(13A)	10132	2482	3570	99
H(13B)	11126	2522	3194	99
H(13C)	11060	2625	4260	99
H(14A)	9892	1778	4726	83
H(14B)	10848	1949	5345	83
H(14C)	10731	1395	4994	83
H(15A)	11726	1218	2784	37
H(34A)	13256	-1550	3465	94
H(34B)	13369	-1037	3996	94
H(34C)	13953	-1142	3160	94
H(35A)	12011	-1139	1311	81
H(35B)	12460	-1609	1861	81
H(35C)	13133	-1196	1533	81
H(36A)	11061	-938	2694	74
H(36B)	11631	-950	3717	74
H(36C)	11494	-1442	3120	74
H(37A)	13870	-337	3406	45
H(40A)	14659	1133	2413	112
H(40B)	15191	1274	3415	112
H(40C)	14070	1331	3190	112
H(41A)	13794	812	4528	97
H(41B)	14911	762	4817	97
H(41C)	14266	283	4679	97

H(42A)	15479	292	2640	95
H(42B)	15345	-30	3526	95
H(42C)	15950	464	3646	95
H(43A)	13029	929	2114	38
H(20E)	12384	1833	-2566	104
H(20F)	12632	1425	-3279	104
H(20G)	13333	1521	-2344	104
H(21A)	13245	606	-2038	87
H(21B)	12487	529	-2940	87
H(21C)	12255	350	-1954	87
H(22A)	10805	1457	-2498	82
H(22B)	10705	884	-2308	82
H(22C)	11041	1068	-3250	82
H(23A)	12962	1847	-1050	43
H(26A)	14457	2092	107	83
H(26B)	14470	1879	1128	83
H(26C)	14647	2450	980	83
H(27A)	12318	2441	1637	81
H(27B)	13339	2686	1873	81
H(27C)	13198	2117	2077	81
H(28A)	12262	2778	8	78
H(28B)	13063	2634	-606	78
H(28C)	13306	2994	259	78
H(29A)	12162	1578	1452	32
H(10A)	10760	2286	346	84
H(10B)	10159	1949	936	84
H(10E)	9801	2754	1208	156
H(10F)	8880	2515	633	156
H(10G)	9548	2862	125	156
H(10C)	9112	2430	-1153	98
H(10D)	9345	1980	-1778	98
H(10H)	10304	2576	-2141	123
H(10I)	10990	2239	-1447	123
H(10J)	10585	2738	-1086	123
H(30A)	9540	-85	4584	122
H(30B)	9604	497	4468	122
H(30C)	9586	461	3152	78
H(30D)	8946	1	3336	78
H(30E)	10021	-79	3183	78
H(30C)	10524	-194	5677	115
H(30D)	10599	-582	4854	115
H(30E)	11983	-635	5871	265
H(30F)	12119	-55	5843	265
H(30G)	12222	-377	4949	265
H(20A)	14619	-230	-245	146
H(20B)	14720	-171	856	146
H(20C)	13216	-115	785	106
H(20D)	13501	-605	292	106
H(20H)	13095	-146	-318	106
H(20C)	15567	252	-396	144
H(20D)	14655	284	-1195	144
H(20H)	15731	1048	-805	336
H(20I)	15014	1122	-69	336
H(20J)	14626	1109	-1150	336

Table 25. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a·6C₇H₆O** (benzaldehyde). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	site occupancy
Na(1)	578(1)	3572(1)	4195(1)	39(1)	
Na(2)	-1834(1)	4275(1)	4833(1)	40(1)	
Na(3)	-147(1)	6235(1)	4233(1)	39(1)	
O(1)	660(2)	4973(2)	3857(1)	35(1)	
O(2)	-965(2)	3191(2)	4424(1)	34(1)	
O(3)	-1601(2)	5690(2)	4454(1)	35(1)	
O(101)	817(2)	2465(2)	3119(2)	58(1)	
O(201)	-3524(2)	3541(3)	4413(2)	84(1)	
O(301)	-344(3)	7129(2)	3415(2)	76(1)	
C(1)	-1513(2)	4111(2)	3217(2)	31(1)	
C(2)	-981(3)	4526(3)	2730(2)	35(1)	
C(3)	124(3)	4901(3)	3082(2)	35(1)	
C(4)	612(3)	5204(3)	2584(2)	40(1)	
C(5)	1799(3)	5603(3)	2916(2)	45(1)	
C(6)	2152(3)	6568(3)	3630(2)	56(1)	
C(7)	2166(3)	5814(4)	2262(2)	63(1)	
C(8)	2348(3)	4873(3)	3201(2)	52(1)	
C(9)	-24(3)	5124(3)	1787(2)	46(1)	
C(10)	-1093(3)	4792(3)	1448(2)	44(1)	
C(11)	-1721(3)	4708(3)	553(2)	54(1)	
C(12)	-1482(4)	3906(4)	-27(2)	71(1)	
C(13)	-2879(4)	4440(5)	335(3)	83(2)	
C(14)	-1408(4)	5666(4)	420(3)	74(1)	
C(15)	-1557(3)	4512(3)	1940(2)	39(1)	
C(16)	-1665(3)	3011(3)	2995(2)	35(1)	
C(17)	-1409(2)	2603(3)	3635(2)	34(1)	
C(18)	-1598(3)	1570(3)	3406(2)	38(1)	
C(19)	-1344(3)	1071(3)	4060(2)	47(1)	
C(20)	-174(3)	1392(3)	4566(2)	55(1)	
C(21)	-1656(4)	-44(3)	3676(3)	71(1)	
C(22)	-1927(3)	1338(3)	4623(2)	58(1)	
C(23)	-2018(3)	1013(3)	2570(2)	43(1)	
C(24)	-2254(3)	1403(3)	1938(2)	42(1)	
C(25)	-2725(3)	727(3)	1034(2)	50(1)	
C(26)	-2935(5)	1273(4)	440(2)	88(2)	
C(27)	-1996(4)	120(4)	873(3)	68(1)	
C(28)	-3761(4)	19(4)	854(3)	74(1)	
C(29)	-2058(3)	2400(3)	2174(2)	40(1)	
C(30)	-2521(2)	4401(2)	3162(2)	32(1)	
C(31)	-2481(2)	5231(2)	3790(2)	31(1)	
C(32)	-3418(3)	5516(3)	3700(2)	36(1)	
C(33)	-3449(3)	6386(3)	4365(2)	47(1)	
C(34)	-2664(3)	7322(3)	4504(3)	62(1)	
C(35)	-4524(3)	6582(4)	4134(3)	68(1)	
C(36)	-3210(3)	6168(3)	5174(2)	60(1)	
C(37)	-4316(3)	4970(3)	3004(2)	41(1)	
C(38)	-4370(3)	4143(3)	2391(2)	39(1)	
C(39)	-5382(3)	3601(3)	1637(2)	49(1)	
C(40)	-5597(5)	4203(5)	1084(3)	103(2)	
C(41)	-5363(4)	2621(4)	1146(3)	106(2)	

C(42)	-6282(4)	3417(5)	1902(4)	111(2)	
C(43)	-3454(3)	3878(3)	2496(2)	37(1)	
C(101)	475(3)	2651(3)	2495(3)	54(1)	
C(102)	648(3)	2258(3)	1741(2)	50(1)	
C(103)	1190(3)	1566(3)	1663(3)	61(1)	
C(104)	1348(4)	1221(4)	952(3)	82(2)	
C(105)	984(5)	1569(5)	327(3)	92(2)	
C(106)	463(5)	2267(5)	399(3)	91(2)	
C(107)	281(4)	2596(4)	1103(3)	75(1)	
C(201)	-4464(6)	3225(5)	4036(4)	115(2)	
C(202)	-4843(4)	2136(5)	3389(3)	89(2)	
C(203)	-5895(7)	1798(6)	3251(5)	127(3)	
C(204)	-6433(5)	793(5)	2607(5)	99(2)	
C(205)	-5787(5)	-417(5)	2277(4)	98(2)	
C(206)	-4733(8)	944(10)	2584(6)	166(5)	
C(207)	-4160(12)	1938(18)	3257(12)	350(16)	
C(301)	-638(5)	7433(5)	2866(3)	89(2)	
C(302)	-1729(4)	7304(4)	2347(3)	67(1)	
C(303)	-1957(5)	7765(4)	1775(3)	80(2)	
C(304)	-2970(5)	7651(4)	1278(4)	94(2)	
C(305)	-3749(6)	7059(6)	1365(4)	125(3)	
C(306)	-3505(6)	6630(6)	1934(5)	130(3)	
C(307)	-2499(5)	6732(4)	2419(4)	88(2)	
C(401)	689(6)	-691(6)	1991(5)	115(2)	
C(402)	1276(8)	-1345(6)	1966(5)	133(3)	
C(403)	1940(7)	-1380(5)	2671(5)	111(2)	
C(404)	2025(5)	-780(6)	3394(4)	104(2)	
C(405)	1445(6)	-149(5)	3427(4)	97(2)	
C(406)	752(6)	-112(5)	2726(5)	99(2)	
C(71)	-5287(13)	10010(12)	5604(9)	106(5)	0.40
C(73)	-4959(14)	9205(9)	4487(9)	107(5)	0.40
C(72A)	-5000	10000	5000	124(16)	0.22
C(74A)	-4350(30)	9240(30)	4090(20)	139(13)	0.22
C(75A)	-4730(30)	8610(30)	3020(20)	129(12)	0.22
C(72B)	-5297(18)	9207(12)	5076(11)	55(6)	0.18
C(74B)	-5220(30)	8800(30)	3686(13)	120(13)	0.18
C(75B)	-5370(40)	8360(30)	2911(18)	110(12)	0.18
C(76B)	-5870(20)	7730(20)	1898(17)	74(7)	0.18

Table 26. Bond lengths [Å] and angles [deg] for **3a·6C₆H₅O** (benzaldehyde).

Na(1)-O(3)#1	2.258(2)	C(24)-C(29)	1.380(5)
Na(1)-O(1)	2.322(3)	C(24)-C(25)	1.538(5)
Na(1)-O(101)	2.371(3)	C(25)-C(26)	1.505(6)
Na(1)-O(2)	2.381(3)	C(25)-C(27)	1.528(6)
Na(1)-C(17)	2.664(4)	C(25)-C(28)	1.544(7)
Na(1)-C(101)	2.997(4)	C(30)-C(43)	1.394(5)
Na(1)-C(16)	3.036(3)	C(30)-C(31)	1.424(4)
Na(1)-Na(3)#1	3.0946(17)	C(31)-C(32)	1.433(4)
Na(1)-Na(2)#1	3.101(2)	C(32)-C(37)	1.397(5)
Na(1)-Na(2)	4.1742(18)	C(32)-C(33)	1.542(5)
Na(2)-O(201)	2.247(3)	C(33)-C(34)	1.540(6)
Na(2)-O(1)#1	2.261(2)	C(33)-C(36)	1.540(6)
Na(2)-O(2)	2.301(3)	C(33)-C(35)	1.543(5)
Na(2)-O(3)	2.391(3)	C(37)-C(38)	1.399(5)
Na(2)-C(31)	2.686(3)	C(38)-C(43)	1.388(5)
Na(2)-C(30)	2.958(3)	C(38)-C(39)	1.531(5)
Na(2)-Na(3)#1	3.0978(18)	C(39)-C(41)	1.505(6)
Na(2)-C(1)	3.100(3)	C(39)-C(40)	1.512(6)
Na(2)-Na(1)#1	3.101(2)	C(39)-C(42)	1.526(7)

Na(2)-Na(3)	4.085(2)	C(101)-C(102)	1.470(5)
Na(3)-O(301)	2.236(3)	C(102)-C(107)	1.373(6)
Na(3)-O(2)#1	2.269(2)	C(102)-C(103)	1.385(5)
Na(3)-O(3)	2.303(3)	C(103)-C(104)	1.376(5)
Na(3)-O(1)	2.416(3)	C(104)-C(105)	1.361(7)
Na(3)-C(3)	2.664(3)	C(105)-C(106)	1.372(7)
Na(3)-C(2)	2.930(4)	C(106)-C(107)	1.380(6)
Na(3)-Na(1)#1	3.0946(17)	C(201)-C(202)	1.608(9)
Na(3)-Na(2)#1	3.0978(18)	C(202)-C(207)	1.141(10)
Na(3)-C(1)	3.114(4)	C(202)-C(203)	1.413(9)
O(1)-C(3)	1.335(4)	C(203)-C(204)	1.517(10)
O(1)-Na(2)#1	2.261(2)	C(204)-C(205)	1.372(9)
O(2)-C(17)	1.341(4)	C(205)-C(206)	1.416(11)
O(2)-Na(3)#1	2.269(2)	C(206)-C(207)	1.53(3)
O(3)-C(31)	1.336(4)	C(301)-C(302)	1.474(7)
O(3)-Na(1)#1	2.258(2)	C(302)-C(307)	1.341(7)
O(101)-C(101)	1.209(5)	C(302)-C(303)	1.380(6)
O(201)-C(201)	1.223(8)	C(303)-C(304)	1.378(8)
O(301)-C(301)	1.190(6)	C(304)-C(305)	1.383(9)
C(1)-C(2)	1.533(4)	C(305)-C(306)	1.342(9)
C(1)-C(16)	1.535(5)	C(306)-C(307)	1.368(9)
C(1)-C(30)	1.542(4)	C(401)-C(406)	1.359(9)
C(2)-C(15)	1.400(4)	C(401)-C(402)	1.379(11)
C(2)-C(3)	1.432(5)	C(402)-C(403)	1.344(10)
C(3)-C(4)	1.437(5)	C(403)-C(404)	1.341(9)
C(4)-C(9)	1.401(5)	C(404)-C(405)	1.348(9)
C(4)-C(5)	1.541(5)	C(405)-C(406)	1.355(9)
C(5)-C(6)	1.535(6)	C(71)-C(73)#2	1.235(17)
C(5)-C(8)	1.536(5)	C(71)-C(72A)	1.302(10)
C(5)-C(7)	1.542(5)	C(71)-C(72B)	1.316(11)
C(9)-C(10)	1.382(5)	C(71)-C(74A)#2	1.37(4)
C(10)-C(15)	1.390(5)	C(71)-C(74B)#2	1.76(4)
C(10)-C(11)	1.546(5)	C(73)-C(71)#2	1.235(17)
C(11)-C(13)	1.518(6)	C(73)-C(74A)	1.316(12)
C(11)-C(14)	1.530(7)	C(73)-C(72B)	1.323(11)
C(11)-C(12)	1.537(6)	C(73)-C(72A)	1.324(10)
C(16)-C(29)	1.398(4)	C(73)-C(74B)	1.325(11)
C(16)-C(17)	1.430(4)	C(72A)-C(71)#2	1.302(10)
C(17)-C(18)	1.432(5)	C(72A)-C(73)#2	1.324(10)
C(18)-C(23)	1.395(5)	C(74A)-C(71)#2	1.37(4)
C(18)-C(19)	1.547(5)	C(74A)-C(75A)	1.78(5)
C(19)-C(20)	1.530(5)	C(74B)-C(75B)	1.323(11)
C(19)-C(21)	1.540(6)	C(74B)-C(71)#2	1.76(4)
C(19)-C(22)	1.541(6)	C(75B)-C(76B)	1.68(4)
C(23)-C(24)	1.398(5)		
O(3)#1-Na(1)-O(1)	96.32(9)	C(30)-C(1)-Na(2)	70.19(15)
O(3)#1-Na(1)-O(101)	131.45(10)	C(2)-C(1)-Na(3)	68.76(18)
O(1)-Na(1)-O(101)	103.30(10)	C(16)-C(1)-Na(3)	150.6(2)
O(3)#1-Na(1)-O(2)	94.21(8)	C(30)-C(1)-Na(3)	92.41(19)
O(1)-Na(1)-O(2)	108.47(9)	Na(2)-C(1)-Na(3)	82.20(8)
O(101)-Na(1)-O(2)	119.80(10)	C(15)-C(2)-C(3)	120.0(3)
O(3)#1-Na(1)-C(17)	123.52(10)	C(15)-C(2)-C(1)	120.9(3)
O(1)-Na(1)-C(17)	108.23(10)	C(3)-C(2)-C(1)	119.1(3)
O(101)-Na(1)-C(17)	91.68(11)	C(15)-C(2)-Na(3)	125.2(2)
O(2)-Na(1)-C(17)	30.17(8)	C(3)-C(2)-Na(3)	65.05(17)
O(3)#1-Na(1)-C(101)	146.63(11)	C(1)-C(2)-Na(3)	82.07(17)
O(1)-Na(1)-C(101)	83.87(11)	O(1)-C(3)-C(2)	119.5(3)
O(101)-Na(1)-C(101)	22.36(10)	O(1)-C(3)-C(4)	122.5(3)
O(2)-Na(1)-C(101)	117.49(10)	C(2)-C(3)-C(4)	118.0(3)
C(17)-Na(1)-C(101)	87.34(11)	O(1)-C(3)-Na(3)	64.68(15)
O(3)#1-Na(1)-C(16)	141.44(9)	C(2)-C(3)-Na(3)	85.78(18)
O(1)-Na(1)-C(16)	83.11(9)	C(4)-C(3)-Na(3)	119.4(2)

O(101)-Na(1)-C(16)	85.36(10)	C(9)-C(4)-C(3)	118.0(3)
O(2)-Na(1)-C(16)	50.74(8)	C(9)-C(4)-C(5)	121.0(3)
C(17)-Na(1)-C(16)	28.10(9)	C(3)-C(4)-C(5)	121.0(3)
C(101)-Na(1)-C(16)	71.87(10)	C(6)-C(5)-C(8)	110.3(3)
O(3)#1-Na(1)-Na(3)#1	47.90(6)	C(6)-C(5)-C(4)	109.3(3)
O(1)-Na(1)-Na(3)#1	113.42(7)	C(8)-C(5)-C(4)	111.2(3)
O(101)-Na(1)-Na(3)#1	143.23(10)	C(6)-C(5)-C(7)	106.8(3)
O(2)-Na(1)-Na(3)#1	46.74(6)	C(8)-C(5)-C(7)	106.5(3)
C(17)-Na(1)-Na(3)#1	75.63(8)	C(4)-C(5)-C(7)	112.6(3)
C(101)-Na(1)-Na(3)#1	158.64(10)	C(10)-C(9)-C(4)	124.6(3)
C(16)-Na(1)-Na(3)#1	96.91(7)	C(9)-C(10)-C(15)	116.9(3)
O(3)#1-Na(1)-Na(2)#1	50.04(7)	C(9)-C(10)-C(11)	120.5(3)
O(1)-Na(1)-Na(2)#1	46.60(6)	C(15)-C(10)-C(11)	122.6(3)
O(101)-Na(1)-Na(2)#1	127.17(9)	C(13)-C(11)-C(14)	108.8(4)
O(2)-Na(1)-Na(2)#1	111.71(7)	C(13)-C(11)-C(12)	108.3(4)
C(17)-Na(1)-Na(2)#1	134.39(9)	C(14)-C(11)-C(12)	109.0(3)
C(101)-Na(1)-Na(2)#1	118.83(10)	C(13)-C(11)-C(10)	111.9(3)
C(16)-Na(1)-Na(2)#1	121.66(8)	C(14)-C(11)-C(10)	110.4(4)
Na(3)#1-Na(1)-Na(2)#1	82.51(5)	C(12)-C(11)-C(10)	108.3(3)
O(3)#1-Na(1)-Na(2)	86.03(6)	C(10)-C(15)-C(2)	122.4(3)
O(1)-Na(1)-Na(2)	84.46(6)	C(29)-C(16)-C(17)	119.4(3)
O(101)-Na(1)-Na(2)	139.21(9)	C(29)-C(16)-C(1)	120.9(3)
O(2)-Na(1)-Na(2)	26.43(6)	C(17)-C(16)-C(1)	119.7(3)
C(17)-Na(1)-Na(2)	48.65(7)	C(29)-C(16)-Na(1)	125.1(2)
C(101)-Na(1)-Na(2)	126.99(9)	C(17)-C(16)-Na(1)	61.36(17)
C(16)-Na(1)-Na(2)	55.46(6)	C(1)-C(16)-Na(1)	84.51(18)
Na(3)#1-Na(1)-Na(2)	47.65(3)	O(2)-C(17)-C(16)	119.6(3)
Na(2)#1-Na(1)-Na(2)	87.31(4)	O(2)-C(17)-C(18)	122.1(3)
O(201)-Na(2)-O(1)#1	127.30(11)	C(16)-C(17)-C(18)	118.3(3)
O(201)-Na(2)-O(2)	111.28(14)	O(2)-C(17)-Na(1)	63.15(16)
O(1)#1-Na(2)-O(2)	97.19(9)	C(16)-C(17)-Na(1)	90.5(2)
O(201)-Na(2)-O(3)	111.09(12)	C(18)-C(17)-Na(1)	114.4(2)
O(1)#1-Na(2)-O(3)	94.31(9)	C(23)-C(18)-C(17)	118.5(3)
O(2)-Na(2)-O(3)	114.60(9)	C(23)-C(18)-C(19)	120.1(3)
O(201)-Na(2)-C(31)	85.38(12)	C(17)-C(18)-C(19)	121.5(3)
O(1)#1-Na(2)-C(31)	122.92(11)	C(20)-C(19)-C(21)	106.8(3)
O(2)-Na(2)-C(31)	113.70(9)	C(20)-C(19)-C(22)	110.5(3)
O(3)-Na(2)-C(31)	29.78(9)	C(21)-C(19)-C(22)	107.7(4)
O(201)-Na(2)-C(30)	82.69(11)	C(20)-C(19)-C(18)	109.3(3)
O(1)#1-Na(2)-C(30)	143.63(11)	C(21)-C(19)-C(18)	112.6(3)
O(2)-Na(2)-C(30)	87.94(9)	C(22)-C(19)-C(18)	109.9(3)
O(3)-Na(2)-C(30)	51.75(9)	C(18)-C(23)-C(24)	124.0(3)
C(31)-Na(2)-C(30)	28.71(9)	C(29)-C(24)-C(23)	116.5(3)
O(201)-Na(2)-Na(3)#1	131.69(12)	C(29)-C(24)-C(25)	123.4(3)
O(1)#1-Na(2)-Na(3)#1	50.71(6)	C(23)-C(24)-C(25)	120.0(3)
O(2)-Na(2)-Na(3)#1	46.88(6)	C(26)-C(25)-C(27)	108.9(4)
O(3)-Na(2)-Na(3)#1	117.22(7)	C(26)-C(25)-C(24)	112.6(3)
C(31)-Na(2)-Na(3)#1	140.33(9)	C(27)-C(25)-C(24)	110.0(3)
C(30)-Na(2)-Na(3)#1	127.77(8)	C(26)-C(25)-C(28)	107.9(4)
O(201)-Na(2)-C(1)	104.47(11)	C(27)-C(25)-C(28)	107.7(4)
O(1)#1-Na(2)-C(1)	128.17(10)	C(24)-C(25)-C(28)	109.7(3)
O(2)-Na(2)-C(1)	61.86(8)	C(24)-C(29)-C(16)	123.4(3)
O(3)-Na(2)-C(1)	60.89(8)	C(43)-C(30)-C(31)	120.3(3)
C(31)-Na(2)-C(1)	51.85(9)	C(43)-C(30)-C(1)	120.7(3)
C(30)-Na(2)-C(1)	29.38(8)	C(31)-C(30)-C(1)	119.0(3)
Na(3)#1-Na(2)-C(1)	98.39(7)	C(43)-C(30)-Na(2)	127.1(2)
O(201)-Na(2)-Na(1)#1	130.82(13)	C(31)-C(30)-Na(2)	64.99(16)
O(1)#1-Na(2)-Na(1)#1	48.26(7)	C(1)-C(30)-Na(2)	80.43(16)
O(2)-Na(2)-Na(1)#1	117.89(8)	O(3)-C(31)-C(30)	119.9(3)
O(3)-Na(2)-Na(1)#1	46.35(6)	O(3)-C(31)-C(32)	122.1(3)
C(31)-Na(2)-Na(1)#1	74.71(8)	C(30)-C(31)-C(32)	117.9(3)
C(30)-Na(2)-Na(1)#1	97.75(8)	O(3)-C(31)-Na(2)	62.78(15)
Na(3)#1-Na(2)-Na(1)#1	86.16(5)	C(30)-C(31)-Na(2)	86.30(19)

C(1)-Na(2)-Na(1)#1	97.63(8)	C(32)-C(31)-Na(2)	119.3(2)
O(201)-Na(2)-Na(3)	135.60(10)	C(37)-C(32)-C(31)	118.5(3)
O(1)#1-Na(2)-Na(3)	86.52(7)	C(37)-C(32)-C(33)	120.3(3)
O(2)-Na(2)-Na(3)	88.08(7)	C(31)-C(32)-C(33)	121.1(3)
O(3)-Na(2)-Na(3)	28.91(5)	C(34)-C(33)-C(36)	110.2(3)
C(31)-Na(2)-Na(3)	50.31(7)	C(34)-C(33)-C(32)	110.9(3)
C(30)-Na(2)-Na(3)	57.57(7)	C(36)-C(33)-C(32)	109.3(3)
Na(3)#1-Na(2)-Na(3)	91.04(4)	C(34)-C(33)-C(35)	107.1(3)
C(1)-Na(2)-Na(3)	49.04(7)	C(36)-C(33)-C(35)	106.7(3)
Na(1)#1-Na(2)-Na(3)	48.68(3)	C(32)-C(33)-C(35)	112.5(3)
O(201)-Na(2)-Na(1)	135.01(12)	C(32)-C(37)-C(38)	124.2(3)
O(1)#1-Na(2)-Na(1)	88.00(7)	C(43)-C(38)-C(37)	116.2(3)
O(2)-Na(2)-Na(1)	27.43(6)	C(43)-C(38)-C(39)	123.1(3)
O(3)-Na(2)-Na(1)	89.74(6)	C(37)-C(38)-C(39)	120.7(3)
C(31)-Na(2)-Na(1)	98.17(7)	C(41)-C(39)-C(40)	108.8(4)
C(30)-Na(2)-Na(1)	80.18(7)	C(41)-C(39)-C(42)	106.2(5)
Na(3)#1-Na(2)-Na(1)	47.58(3)	C(40)-C(39)-C(42)	109.0(5)
C(1)-Na(2)-Na(1)	50.81(6)	C(41)-C(39)-C(38)	112.9(3)
Na(1)#1-Na(2)-Na(1)	92.69(4)	C(40)-C(39)-C(38)	109.5(4)
Na(3)-Na(2)-Na(1)	61.66(3)	C(42)-C(39)-C(38)	110.3(3)
O(301)-Na(3)-O(2)#1	123.73(12)	C(38)-C(43)-C(30)	122.9(3)
O(301)-Na(3)-O(3)	114.89(12)	O(101)-C(101)-C(102)	125.8(4)
O(2)#1-Na(3)-O(3)	96.06(9)	O(101)-C(101)-Na(1)	48.3(2)
O(301)-Na(3)-O(1)	112.80(11)	C(102)-C(101)-Na(1)	168.7(3)
O(2)#1-Na(3)-O(1)	93.79(9)	C(107)-C(102)-C(103)	119.1(4)
O(3)-Na(3)-O(1)	113.18(10)	C(107)-C(102)-C(101)	119.2(4)
O(301)-Na(3)-C(3)	87.92(12)	C(103)-C(102)-C(101)	121.7(4)
O(2)#1-Na(3)-C(3)	122.64(10)	C(104)-C(103)-C(102)	120.2(4)
O(3)-Na(3)-C(3)	113.12(11)	C(105)-C(104)-C(103)	120.0(4)
O(1)-Na(3)-C(3)	29.97(8)	C(104)-C(105)-C(106)	120.7(4)
O(301)-Na(3)-C(2)	86.92(11)	C(105)-C(106)-C(107)	119.4(5)
O(2)#1-Na(3)-C(2)	143.04(10)	C(102)-C(107)-C(106)	120.6(4)
O(3)-Na(3)-C(2)	87.15(9)	O(201)-C(201)-C(202)	114.5(7)
O(1)-Na(3)-C(2)	52.06(8)	C(207)-C(202)-C(203)	145.5(15)
C(3)-Na(3)-C(2)	29.17(10)	C(207)-C(202)-C(201)	109.4(14)
O(301)-Na(3)-Na(1)#1	131.42(10)	C(203)-C(202)-C(201)	105.0(7)
O(2)#1-Na(3)-Na(1)#1	49.84(6)	C(202)-C(203)-C(204)	113.8(6)
O(3)-Na(3)-Na(1)#1	46.65(6)	C(205)-C(204)-C(203)	112.2(6)
O(1)-Na(3)-Na(1)#1	115.61(7)	C(204)-C(205)-C(206)	119.6(7)
C(3)-Na(3)-Na(1)#1	139.14(9)	C(205)-C(206)-C(207)	129.2(11)
C(2)-Na(3)-Na(1)#1	126.66(8)	C(202)-C(207)-C(206)	99.1(16)
O(301)-Na(3)-Na(2)#1	128.76(11)	O(301)-C(301)-C(302)	125.9(5)
O(2)#1-Na(3)-Na(2)#1	47.76(6)	C(307)-C(302)-C(303)	119.8(5)
O(3)-Na(3)-Na(2)#1	116.27(7)	C(307)-C(302)-C(301)	120.6(5)
O(1)-Na(3)-Na(2)#1	46.41(6)	C(303)-C(302)-C(301)	119.6(5)
C(3)-Na(3)-Na(2)#1	74.91(8)	C(304)-C(303)-C(302)	120.8(6)
C(2)-Na(3)-Na(2)#1	98.08(8)	C(303)-C(304)-C(305)	118.3(6)
Na(1)#1-Na(3)-Na(2)#1	84.77(4)	C(306)-C(305)-C(304)	119.6(7)
O(301)-Na(3)-C(1)	109.49(11)	C(305)-C(306)-C(307)	122.0(7)
O(2)#1-Na(3)-C(1)	126.69(10)	C(302)-C(307)-C(306)	119.4(6)
O(3)-Na(3)-C(1)	61.32(8)	C(406)-C(401)-C(402)	120.0(7)
O(1)-Na(3)-C(1)	60.36(8)	C(403)-C(402)-C(401)	119.8(7)
C(3)-Na(3)-C(1)	51.81(10)	C(404)-C(403)-C(402)	119.7(7)
C(2)-Na(3)-C(1)	29.18(8)	C(403)-C(404)-C(405)	121.1(7)
Na(1)#1-Na(3)-C(1)	97.48(7)	C(404)-C(405)-C(406)	120.5(6)
Na(2)#1-Na(3)-C(1)	96.97(7)	C(405)-C(406)-C(401)	118.8(7)
O(301)-Na(3)-Na(2)	141.22(11)	C(73)#2-C(71)-C(72A)	62.9(6)
O(2)#1-Na(3)-Na(2)	86.62(7)	C(73)#2-C(71)-C(72B)	119.7(8)
O(3)-Na(3)-Na(2)	30.13(6)	C(72A)-C(71)-C(72B)	56.9(9)
O(1)-Na(3)-Na(2)	85.40(7)	C(73)#2-C(71)-C(74A)#2	60.4(12)
C(3)-Na(3)-Na(2)	95.04(9)	C(72A)-C(71)-C(74A)#2	119.1(16)
C(2)-Na(3)-Na(2)	77.90(7)	C(72B)-C(71)-C(74A)#2	157(3)
Na(1)#1-Na(3)-Na(2)	48.81(4)	C(73)#2-C(71)-C(74B)#2	48.7(13)

Na(2)#1-Na(3)-Na(2)	88.96(4)	C(72A)-C(71)-C(74B)#2	107.0(15)
C(1)-Na(3)-Na(2)	48.76(6)	C(72B)-C(71)-C(74B)#2	157(2)
C(3)-O(1)-Na(2)#1	155.7(2)	C(74A)#2-C(71)-C(74B)#2	42(2)
C(3)-O(1)-Na(1)	118.8(2)	C(71)#2-C(73)-C(74A)	65(2)
Na(2)#1-O(1)-Na(1)	85.13(8)	C(71)#2-C(73)-C(72B)	117.2(8)
C(3)-O(1)-Na(3)	85.35(17)	C(74A)-C(73)-C(72B)	162(3)
Na(2)#1-O(1)-Na(3)	82.89(8)	C(71)#2-C(73)-C(72A)	61.0(6)
Na(1)-O(1)-Na(3)	126.62(10)	C(74A)-C(73)-C(72A)	122(2)
C(17)-O(2)-Na(3)#1	157.9(2)	C(72B)-C(73)-C(72A)	56.2(9)
C(17)-O(2)-Na(2)	116.32(18)	C(71)#2-C(73)-C(74B)	87(2)
Na(3)#1-O(2)-Na(2)	85.36(8)	C(74A)-C(73)-C(74B)	53(2)
C(17)-O(2)-Na(1)	86.69(17)	C(72B)-C(73)-C(74B)	142(3)
Na(3)#1-O(2)-Na(1)	83.42(8)	C(72A)-C(73)-C(74B)	138(2)
Na(2)-O(2)-Na(1)	126.14(11)	C(71)#2-C(72A)-C(71)	180.000(9)
C(31)-O(3)-Na(1)#1	157.14(19)	C(71)#2-C(72A)-C(73)#2	123.9(9)
C(31)-O(3)-Na(3)	117.07(18)	C(71)-C(72A)-C(73)#2	56.1(9)
Na(1)#1-O(3)-Na(3)	85.45(9)	C(71)#2-C(72A)-C(73)	56.1(9)
C(31)-O(3)-Na(2)	87.44(18)	C(71)-C(72A)-C(73)	123.9(9)
Na(1)#1-O(3)-Na(2)	83.61(8)	C(73)#2-C(72A)-C(73)	180.000(7)
Na(3)-O(3)-Na(2)	120.96(10)	C(73)-C(74A)-C(71)#2	54.7(12)
C(101)-O(101)-Na(1)	109.4(3)	C(73)-C(74A)-C(75A)	124(3)
C(201)-O(201)-Na(2)	164.8(4)	C(71)#2-C(74A)-C(75A)	124(3)
C(301)-O(301)-Na(3)	165.3(4)	C(71)-C(72B)-C(73)	122.8(12)
C(2)-C(1)-C(16)	111.7(2)	C(75B)-C(74B)-C(73)	173(5)
C(2)-C(1)-C(30)	113.1(3)	C(75B)-C(74B)-C(71)#2	137(4)
C(16)-C(1)-C(30)	112.6(3)	C(73)-C(74B)-C(71)#2	44.5(12)
C(2)-C(1)-Na(2)	150.8(2)	C(74B)-C(75B)-C(76B)	166(4)
C(16)-C(1)-Na(2)	91.81(17)		

Symmetry transformations used to generate equivalent atoms:

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

Table 27. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a-6C₇H₆O** (benzaldehyde). The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Na(1)	39(1)	57(1)	25(1)	14(1)	15(1)	22(1)
Na(2)	40(1)	56(1)	28(1)	17(1)	14(1)	23(1)
Na(3)	37(1)	60(1)	24(1)	13(1)	13(1)	23(1)
O(1)	35(1)	57(2)	21(1)	16(1)	14(1)	22(1)
O(2)	35(1)	50(1)	19(1)	12(1)	9(1)	18(1)
O(3)	33(1)	53(2)	22(1)	12(1)	12(1)	23(1)
O(101)	60(2)	75(2)	40(2)	11(1)	24(1)	29(2)
O(201)	44(2)	133(3)	59(2)	39(2)	10(2)	-3(2)
O(301)	108(3)	82(2)	49(2)	36(2)	25(2)	46(2)
C(1)	32(2)	49(2)	17(1)	10(1)	11(1)	21(2)
C(2)	40(2)	51(2)	23(2)	16(2)	16(1)	26(2)
C(3)	37(2)	56(2)	20(2)	13(2)	15(1)	26(2)
C(4)	46(2)	59(2)	29(2)	20(2)	22(2)	29(2)
C(5)	45(2)	67(3)	34(2)	20(2)	22(2)	21(2)
C(6)	57(3)	71(3)	49(2)	25(2)	28(2)	15(2)
C(7)	53(3)	103(4)	44(2)	32(2)	30(2)	22(2)
C(8)	39(2)	80(3)	48(2)	28(2)	23(2)	26(2)
C(9)	57(2)	72(3)	30(2)	28(2)	29(2)	35(2)
C(10)	50(2)	73(3)	29(2)	26(2)	23(2)	38(2)

C(11)	59(2)	94(3)	28(2)	32(2)	21(2)	43(2)
C(12)	95(4)	105(4)	28(2)	28(2)	25(2)	54(3)
C(13)	62(3)	171(6)	37(2)	56(3)	19(2)	54(3)
C(14)	94(4)	109(4)	44(2)	50(3)	30(2)	52(3)
C(15)	42(2)	61(2)	26(2)	20(2)	18(2)	27(2)
C(16)	34(2)	51(2)	24(2)	12(2)	13(1)	23(2)
C(17)	29(2)	52(2)	23(2)	12(2)	11(1)	19(2)
C(18)	37(2)	49(2)	28(2)	12(2)	10(2)	19(2)
C(19)	55(2)	52(2)	34(2)	16(2)	12(2)	23(2)
C(20)	60(3)	68(3)	37(2)	19(2)	8(2)	35(2)
C(21)	96(4)	55(3)	48(2)	20(2)	9(2)	24(3)
C(22)	64(3)	72(3)	44(2)	29(2)	24(2)	16(2)
C(23)	47(2)	45(2)	35(2)	10(2)	13(2)	24(2)
C(24)	43(2)	53(2)	26(2)	7(2)	9(2)	24(2)
C(25)	54(2)	60(3)	29(2)	7(2)	8(2)	27(2)
C(26)	137(5)	87(4)	27(2)	10(2)	17(3)	50(4)
C(27)	76(3)	77(3)	41(2)	0(2)	20(2)	37(3)
C(28)	59(3)	92(4)	46(2)	1(2)	3(2)	31(3)
C(29)	42(2)	60(2)	23(2)	16(2)	11(2)	28(2)
C(30)	35(2)	47(2)	23(2)	16(1)	14(1)	22(2)
C(31)	28(2)	50(2)	22(2)	15(2)	11(1)	18(2)
C(32)	34(2)	49(2)	29(2)	13(2)	14(2)	21(2)
C(33)	35(2)	64(3)	40(2)	9(2)	12(2)	28(2)
C(34)	53(3)	58(3)	64(3)	6(2)	16(2)	29(2)
C(35)	50(3)	82(3)	63(3)	-1(2)	20(2)	40(2)
C(36)	52(2)	90(3)	39(2)	6(2)	25(2)	33(2)
C(37)	32(2)	58(2)	37(2)	17(2)	13(2)	22(2)
C(38)	37(2)	57(2)	29(2)	17(2)	12(2)	24(2)
C(39)	39(2)	62(3)	36(2)	12(2)	5(2)	21(2)
C(40)	90(4)	110(5)	64(3)	41(3)	-25(3)	11(3)
C(41)	77(4)	86(4)	75(3)	-21(3)	-37(3)	42(3)
C(42)	47(3)	156(6)	81(4)	-4(4)	20(3)	-14(3)
C(43)	41(2)	52(2)	23(2)	15(2)	13(1)	24(2)
C(101)	50(2)	64(3)	50(2)	10(2)	23(2)	29(2)
C(102)	50(2)	64(3)	36(2)	10(2)	18(2)	27(2)
C(103)	67(3)	84(3)	48(2)	24(2)	30(2)	48(2)
C(104)	111(4)	113(4)	55(3)	31(3)	48(3)	78(4)
C(105)	118(5)	130(5)	47(3)	24(3)	41(3)	77(4)
C(106)	128(5)	122(5)	40(3)	31(3)	32(3)	72(4)
C(107)	87(4)	94(4)	52(3)	22(3)	26(2)	56(3)
C(202)	61(3)	110(5)	57(3)	45(3)	-14(3)	-25(3)
C(203)	158(7)	123(6)	187(8)	83(6)	128(7)	89(6)
C(204)	65(3)	103(5)	146(6)	79(5)	32(4)	32(3)
C(205)	89(5)	90(4)	89(4)	12(3)	19(4)	21(4)
C(206)	106(7)	286(14)	118(7)	78(8)	59(6)	38(8)
C(207)	287(16)	800(40)	470(30)	590(30)	343(19)	450(20)
C(301)	89(4)	108(5)	82(4)	56(4)	31(3)	31(3)
C(302)	87(4)	68(3)	53(3)	28(2)	28(3)	27(3)
C(303)	87(4)	79(4)	64(3)	33(3)	12(3)	16(3)
C(304)	105(5)	83(4)	76(4)	30(3)	9(3)	30(4)
C(305)	96(5)	146(7)	101(5)	53(5)	4(4)	12(5)
C(306)	106(6)	150(7)	115(6)	68(5)	20(5)	-4(5)
C(307)	92(4)	89(4)	79(4)	34(3)	29(3)	18(3)
C(401)	97(5)	133(7)	88(5)	35(5)	16(4)	11(5)
C(402)	172(9)	98(6)	105(6)	6(5)	54(6)	29(6)
C(403)	155(7)	93(5)	130(6)	60(5)	82(6)	60(5)
C(404)	112(5)	144(6)	88(5)	65(5)	50(4)	54(5)
C(405)	121(5)	98(5)	79(4)	25(3)	52(4)	31(4)
C(406)	120(5)	96(5)	112(5)	48(4)	62(5)	50(4)

Table 28. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**·6C₆H₅O (benzaldehyde).

	x	y	z	U(eq)
H(1A)	-1033	4405	3797	38
H(6A)	1935	6470	4052	84
H(6B)	1850	7035	3433	84
H(6C)	2894	6805	3853	84
H(7A)	1960	5226	1803	94
H(7B)	2907	6060	2498	94
H(7C)	1860	6287	2080	94
H(8A)	2141	4719	3610	78
H(8B)	3085	5153	3431	78
H(8C)	2163	4292	2739	78
H(9A)	296	5308	1462	55
H(12A)	-753	4070	94	107
H(12B)	-1861	3846	-587	107
H(12C)	-1682	3300	49	107
H(13A)	-3043	4933	693	124
H(13B)	-3087	3829	402	124
H(13C)	-3242	4387	-226	124
H(14A)	-678	5835	544	111
H(14B)	-1563	6169	775	111
H(14C)	-1786	5597	-143	111
H(15A)	-2277	4309	1736	47
H(20A)	52	2085	4824	83
H(20B)	177	1197	4210	83
H(20C)	-16	1095	4981	83
H(21A)	-1491	-319	4105	106
H(21B)	-1285	-232	3336	106
H(21C)	-2388	-275	3347	106
H(22A)	-1742	2031	4876	87
H(22B)	-1743	1050	5043	87
H(22C)	-2661	1100	4303	87
H(23A)	-2149	343	2426	51
H(26A)	-2300	1718	540	132
H(26B)	-3424	1627	516	132
H(26C)	-3216	822	-113	132
H(27A)	-1343	543	980	102
H(27B)	-2298	-305	309	102
H(27C)	-1888	-258	1228	102
H(28A)	-3648	-336	1229	111
H(28B)	-4032	-427	299	111
H(28C)	-4247	379	922	111
H(29A)	-2195	2679	1766	48
H(34A)	-1984	7225	4644	92
H(34B)	-2664	7844	4944	92
H(34C)	-2855	7480	4009	92
H(35A)	-4702	6726	3633	103
H(35B)	-4507	7124	4567	103
H(35C)	-5033	6017	4057	103
H(36A)	-2543	6044	5342	90
H(36B)	-3730	5608	5089	90
H(36C)	-3208	6716	5594	90
H(37A)	-4916	5169	2944	49
H(40A)	-5043	4306	902	154
H(40B)	-5646	4819	1384	154
H(40C)	-6237	3868	616	154
H(41A)	-4803	2697	967	159

H(41B)	-6007	2321	675	159
H(41C)	-5267	2219	1482	159
H(42A)	-6911	3072	1425	167
H(42B)	-6353	4026	2194	167
H(42C)	-6150	3037	2256	167
H(43A)	-3464	3327	2104	44
H(10A)	67	3081	2493	64
H(10B)	1448	1334	2092	73
H(10C)	1704	750	898	99
H(10D)	1090	1330	-153	110
H(10E)	235	2517	-22	109
H(10F)	-95	3052	1146	90
H(20F)	-4921	3584	4116	138
H(20D)	-6227	2158	3528	152
H(20G)	-7122	469	2454	118
H(20I)	-6039	-180	1854	117
H(20E)	-4333	644	2342	199
H(20H)	-3462	2278	3490	420
H(30A)	-134	7785	2754	106
H(30B)	-1422	8158	1724	96
H(30C)	-3125	7963	893	113
H(30D)	-4439	6959	1031	149
H(30E)	-4036	6252	2002	156
H(30F)	-2350	6407	2794	105
H(40D)	251	-646	1504	138
H(40E)	1212	-1761	1462	159
H(40F)	2338	-1819	2658	133
H(40G)	2493	-800	3881	124
H(40H)	1521	266	3935	116
H(40I)	328	301	2748	119

Table 29. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**·**6C**₉H₈O (*trans*-Cinnamaldehyde). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)	Site Occupancy
Na(1)	5803(1)	658(1)	9265(1)	28(1)	
Na(2)	3467(1)	1173(1)	9950(1)	28(1)	
Na(3)	5742(1)	-328(1)	11022(1)	27(1)	
O(1)	6467(1)	2(1)	10203(1)	25(1)	
O(2)	4282(1)	1408(1)	9244(1)	25(1)	
O(3)	4271(1)	477(1)	10888(1)	24(1)	
C(1)	5015(2)	1497(2)	10258(1)	20(1)	
C(2)	5908(2)	1203(2)	10565(1)	22(1)	
C(3)	6610(2)	471(2)	10492(1)	24(1)	
C(4)	7444(2)	246(2)	10753(1)	28(1)	
C(5)	8234(2)	-534(2)	10690(1)	35(1)	
C(6)	9072(2)	-629(2)	10974(2)	55(1)	
C(7)	8335(2)	-470(2)	10046(2)	47(1)	
C(8)	8151(2)	-1333(2)	10986(2)	44(1)	
C(9)	7525(2)	749(2)	11068(1)	33(1)	
C(10)	6840(2)	1452(2)	11161(1)	30(1)	
C(11)	6986(2)	1964(2)	11529(1)	36(1)	

C(12)	6142(2)	2664(2)	11611(2)	49(1)
C(13)	7527(3)	2374(3)	11224(2)	58(1)
C(14)	7448(3)	1380(2)	12129(2)	53(1)
C(15)	6037(2)	1661(2)	10905(1)	27(1)
C(16)	4824(2)	2149(2)	9671(1)	22(1)
C(17)	4416(2)	2082(2)	9193(1)	22(1)
C(18)	4189(2)	2737(2)	8657(1)	29(1)
C(19)	3749(2)	2700(2)	8121(1)	37(1)
C(20)	4356(3)	1935(2)	7925(1)	46(1)
C(21)	3521(3)	3486(2)	7605(2)	58(1)
C(22)	2914(2)	2661(2)	8260(2)	49(1)
C(23)	4370(2)	3408(2)	8631(1)	33(1)
C(24)	4789(2)	3474(2)	9097(1)	30(1)
C(25)	4930(2)	4255(2)	9042(2)	40(1)
C(26)	5492(3)	4150(2)	9568(2)	56(1)
C(27)	4056(3)	5017(2)	8996(2)	63(1)
C(28)	5352(3)	4431(2)	8498(2)	57(1)
C(29)	5019(2)	2826(2)	9607(1)	26(1)
C(30)	4309(2)	1800(2)	10644(1)	21(1)
C(31)	4002(2)	1240(2)	10964(1)	22(1)
C(32)	3387(2)	1538(2)	11351(1)	26(1)
C(33)	3016(2)	970(2)	11709(1)	34(1)
C(34)	3735(2)	141(2)	12094(2)	44(1)
C(35)	2397(2)	1390(2)	12112(2)	47(1)
C(36)	2511(2)	780(2)	11293(2)	44(1)
C(37)	3121(2)	2350(2)	11391(1)	29(1)
C(38)	3394(2)	2918(2)	11064(1)	29(1)
C(39)	3076(2)	3804(2)	11135(1)	34(1)
C(40)	3371(3)	4356(2)	10687(2)	59(1)
C(41)	3432(2)	3730(2)	11744(2)	50(1)
C(42)	2098(2)	4256(2)	11068(2)	41(1)
C(43)	3982(2)	2625(2)	10688(1)	26(1)
O(101)	6540(2)	1425(2)	8900(1)	54(1)
C(101)	6867(2)	1685(2)	9194(2)	49(1)
C(102)	7355(2)	2141(2)	8976(2)	46(1)
C(103)	7813(2)	2285(2)	9333(2)	49(1)
C(104)	8389(2)	2669(2)	9178(2)	49(1)
C(105)	8497(4)	2961(3)	8613(2)	76(1)
C(106)	9076(4)	3293(4)	8483(2)	92(2)
C(107)	9522(3)	3362(3)	8909(2)	72(1)
C(108)	9411(4)	3088(4)	9460(3)	97(2)
C(109)	8854(4)	2746(4)	9598(2)	85(2)
O(201)	2273(2)	2449(2)	9849(1)	54(1)
C(201)	2309(2)	3107(2)	9660(2)	48(1)
C(202)	1579(2)	3937(2)	9542(2)	46(1)
C(203)	1676(2)	4634(2)	9342(2)	46(1)
C(204)	1023(2)	5513(2)	9218(2)	41(1)
C(205)	1274(2)	6152(2)	9085(2)	44(1)
C(206)	682(2)	6986(2)	8974(2)	50(1)
C(207)	-173(2)	7199(2)	8989(2)	50(1)
C(208)	-435(2)	6576(2)	9118(2)	53(1)
C(209)	154(2)	5739(2)	9229(2)	49(1)
O(301)	5995(2)	-168(2)	11920(1)	46(1)
C(301)	5591(2)	468(2)	12066(1)	41(1)
C(302)	5673(2)	545(2)	12647(1)	42(1)
C(303)	5158(2)	1237(2)	12783(1)	39(1)
C(304)	5162(2)	1407(2)	13345(1)	39(1)
C(305)	5853(2)	917(3)	13782(2)	51(1)
C(306)	5830(3)	1095(3)	14309(2)	62(1)
C(307)	5122(3)	1752(3)	14412(2)	58(1)
C(308)	4439(2)	2234(2)	13988(2)	52(1)
C(309)	4460(2)	2068(2)	13455(2)	46(1)
Na(1B)	10930(1)	5411(1)	4266(1)	28(1)

Na (2B)	10754 (1)	4677 (1)	6011 (1)	29 (1)
Na (3B)	8562 (1)	6353 (1)	4864 (1)	28 (1)
O (1B)	9497 (1)	6359 (1)	4156 (1)	26 (1)
O (2B)	11535 (1)	4790 (1)	5258 (1)	25 (1)
O (3B)	9295 (1)	5706 (1)	5780 (1)	25 (1)
C (1B)	10266 (2)	6470 (2)	5155 (1)	19 (1)
C (2B)	9678 (2)	7245 (2)	4662 (1)	22 (1)
C (3B)	9353 (2)	7130 (2)	4167 (1)	22 (1)
C (4B)	8855 (2)	7869 (2)	3698 (1)	27 (1)
C (5B)	8443 (2)	7810 (2)	3161 (1)	36 (1)
C (6B)	9113 (2)	7217 (2)	2859 (1)	43 (1)
C (7B)	7981 (3)	8668 (2)	2699 (2)	55 (1)
C (8B)	7777 (2)	7494 (3)	3352 (2)	49 (1)
C (9B)	8719 (2)	8657 (2)	3747 (1)	30 (1)
C (10B)	9016 (2)	8773 (2)	4235 (1)	26 (1)
C (11B)	8863 (2)	9639 (2)	4293 (1)	34 (1)
C (12B)	8438 (3)	9775 (2)	4843 (2)	64 (1)
C (13B)	8290 (2)	10365 (2)	3773 (2)	43 (1)
C (14B)	9718 (2)	9667 (2)	4346 (2)	48 (1)
C (15B)	9484 (2)	8053 (2)	4687 (1)	24 (1)
C (16B)	11214 (2)	6235 (2)	5113 (1)	21 (1)
C (17B)	11811 (2)	5375 (2)	5191 (1)	22 (1)
C (18B)	12695 (2)	5174 (2)	5177 (1)	26 (1)
C (19B)	13377 (2)	4262 (2)	5271 (2)	36 (1)
C (20B)	13243 (2)	3934 (2)	4775 (2)	50 (1)
C (21B)	14287 (2)	4173 (2)	5285 (2)	53 (1)
C (22B)	13338 (2)	3702 (2)	5854 (2)	49 (1)
C (23B)	12927 (2)	5830 (2)	5059 (1)	30 (1)
C (24B)	12349 (2)	6674 (2)	4959 (1)	28 (1)
C (25B)	12611 (2)	7392 (2)	4832 (2)	36 (1)
C (26B)	12100 (2)	8065 (2)	4270 (2)	57 (1)
C (27B)	12433 (2)	7792 (2)	5335 (2)	51 (1)
C (28B)	13558 (2)	7079 (2)	4765 (2)	50 (1)
C (29B)	11497 (2)	6853 (2)	4991 (1)	24 (1)
C (30B)	10003 (2)	6568 (2)	5751 (1)	22 (1)
C (31B)	9484 (2)	6195 (2)	6022 (1)	22 (1)
C (32B)	9208 (2)	6338 (2)	6559 (1)	28 (1)
C (33B)	8684 (2)	5924 (2)	6893 (1)	37 (1)
C (34B)	7835 (2)	6222 (2)	6521 (2)	48 (1)
C (35B)	8465 (3)	6157 (3)	7464 (2)	61 (1)
C (36B)	9198 (2)	4964 (2)	7057 (1)	43 (1)
C (37B)	9419 (2)	6862 (2)	6780 (1)	33 (1)
C (38B)	9938 (2)	7223 (2)	6526 (1)	29 (1)
C (39B)	10118 (2)	7809 (2)	6796 (1)	36 (1)
C (40B)	9290 (3)	8633 (2)	6707 (2)	56 (1)
C (41B)	10804 (2)	8023 (2)	6519 (2)	44 (1)
C (42B)	10416 (3)	7404 (3)	7449 (2)	55 (1)
C (43B)	10237 (2)	7041 (2)	6019 (1)	24 (1)
O (401)	11423 (2)	6239 (2)	3616 (1)	59 (1)
C (401)	11090 (2)	7005 (3)	3526 (2)	50 (1)
C (402)	11137 (3)	7594 (2)	3014 (2)	53 (1)
C (403)	10667 (2)	8419 (2)	2922 (2)	47 (1)
C (404)	10605 (2)	9097 (2)	2422 (2)	44 (1)
C (405)	10050 (3)	9919 (3)	2383 (2)	70 (1)
C (406)	9966 (4)	10573 (3)	1909 (2)	78 (1)
C (407)	10445 (3)	10415 (3)	1459 (2)	64 (1)
C (408)	10973 (4)	9611 (3)	1484 (3)	102 (2)
C (409)	11061 (4)	8956 (3)	1965 (2)	96 (2)
O (501)	11256 (2)	4841 (2)	6810 (1)	50 (1)
C (501)	11555 (2)	5233 (2)	6993 (2)	46 (1)
C (502)	12188 (2)	5468 (2)	6740 (2)	45 (1)
C (503)	12585 (2)	5763 (2)	7024 (2)	48 (1)
C (504)	13298 (3)	5936 (2)	6863 (2)	51 (1)

C(505)	13465(4)	6487(3)	7082(2)	81(2)	
C(506)	14122(4)	6673(4)	6929(3)	101(2)	
C(507)	14643(4)	6297(4)	6553(3)	97(2)	
C(508)	14501(3)	5740(3)	6329(2)	82(2)	
C(509)	13828(3)	5566(3)	6483(2)	63(1)	
O(601)	7497(2)	7609(2)	4960(1)	54(1)	
C(601)	7582(2)	8008(2)	5264(2)	46(1)	
C(602)	6887(2)	8708(2)	5402(2)	44(1)	
C(603)	7026(2)	9108(2)	5748(2)	46(1)	
C(604)	6398(3)	9826(2)	5921(2)	50(1)	
C(605)	5532(3)	10069(3)	5842(2)	64(1)	
C(606)	4957(4)	10762(3)	6010(2)	88(2)	
C(607)	5253(5)	11209(3)	6249(2)	99(2)	
C(608)	6122(5)	10963(3)	6327(2)	99(2)	
C(609)	6690(4)	10273(3)	6173(2)	72(1)	
O(91)	13148(3)	6773(3)	2548(2)	28(1)	0.5
C(91)	13478(4)	5927(4)	2853(3)	45(2)	0.5
C(92)	13072(4)	5521(4)	2675(4)	54(2)	0.5
C(93A)	13293(12)	7278(12)	2767(7)	180(30)	0.25
C(93B)	13715(9)	7115(8)	2628(9)	64(6)	0.25
C(94A)	14005(12)	7221(12)	2818(14)	100(9)	0.25
C(94B)	13351(15)	7879(13)	2602(7)	124(14)	0.25

Table 30. Bond lengths [Å] and angles [deg] for **3a·6C₉H₈O** (trans-Cinnamaldehyde).

Na(1)-O(3)#1	2.271(2)	C(18)-C(23)	1.392(4)
Na(1)-O(1)	2.307(2)	C(18)-C(19)	1.541(4)
Na(1)-O(101)	2.326(3)	C(19)-C(22)	1.534(5)
Na(1)-O(2)	2.407(2)	C(19)-C(21)	1.541(4)
Na(1)-C(17)	2.651(3)	C(19)-C(20)	1.540(5)
Na(1)-C(16)	2.948(3)	C(23)-C(24)	1.405(4)
Na(1)-Na(2)#1	3.0924(15)	C(24)-C(29)	1.389(4)
Na(1)-Na(3)#1	3.1475(15)	C(24)-C(25)	1.538(4)
Na(1)-Na(3)	4.1797(15)	C(25)-C(26)	1.530(5)
Na(2)-O(1)#1	2.241(2)	C(25)-C(28)	1.536(5)
Na(2)-O(2)	2.299(2)	C(25)-C(27)	1.543(5)
Na(2)-O(201)	2.320(3)	C(30)-C(43)	1.403(4)
Na(2)-O(3)	2.388(2)	C(30)-C(31)	1.424(4)
Na(2)-C(31)	2.674(3)	C(31)-C(32)	1.440(4)
Na(2)-C(30)	2.973(3)	C(32)-C(37)	1.390(4)
Na(2)-Na(1)#1	3.0924(15)	C(32)-C(33)	1.547(4)
Na(2)-C(201)	3.118(4)	C(33)-C(35)	1.538(4)
Na(2)-C(17)	3.126(3)	C(33)-C(36)	1.541(5)
Na(2)-Na(3)#1	3.1301(15)	C(33)-C(34)	1.544(5)
Na(2)-Na(3)	4.1312(15)	C(37)-C(38)	1.400(4)
Na(3)-O(2)#1	2.258(2)	C(38)-C(43)	1.391(4)
Na(3)-O(3)	2.323(2)	C(38)-C(39)	1.534(4)
Na(3)-O(301)	2.328(2)	C(39)-C(42)	1.535(4)
Na(3)-O(1)	2.436(2)	C(39)-C(40)	1.538(4)
Na(3)-C(3)	2.666(3)	C(39)-C(41)	1.545(5)
Na(3)-C(2)	2.894(3)	O(101)-C(101)	1.216(5)
Na(3)-C(1)	3.067(3)	C(101)-C(102)	1.456(5)
Na(3)-C(31)	3.127(3)	C(102)-C(103)	1.332(5)
Na(3)-Na(2)#1	3.1301(15)	C(103)-C(104)	1.468(5)
Na(3)-Na(1)#1	3.1475(15)	C(104)-C(105)	1.375(6)
O(1)-C(3)	1.339(3)	C(104)-C(109)	1.377(6)
O(1)-Na(2)#1	2.241(2)	C(105)-C(106)	1.398(6)
O(2)-C(17)	1.337(3)	C(106)-C(107)	1.357(7)
O(2)-Na(3)#1	2.258(2)	C(107)-C(108)	1.342(7)
O(3)-C(31)	1.335(3)	C(108)-C(109)	1.377(7)

O(3)-Na(1)#1	2.271(2)	O(201)-C(201)	1.211(4)
C(1)-C(16)	1.529(3)	C(201)-C(202)	1.459(5)
C(1)-C(30)	1.537(3)	C(202)-C(203)	1.337(5)
C(1)-C(2)	1.539(3)	C(203)-C(204)	1.468(5)
C(2)-C(15)	1.400(4)	C(204)-C(205)	1.394(5)
C(2)-C(3)	1.427(4)	C(204)-C(209)	1.400(5)
C(3)-C(4)	1.436(4)	C(205)-C(206)	1.382(5)
C(4)-C(9)	1.391(4)	C(206)-C(207)	1.380(5)
C(4)-C(5)	1.542(4)	C(207)-C(208)	1.380(5)
C(5)-C(8)	1.531(5)	C(208)-C(209)	1.384(5)
C(5)-C(7)	1.542(5)	O(301)-C(301)	1.217(4)
C(5)-C(6)	1.548(4)	C(301)-C(302)	1.457(4)
C(9)-C(10)	1.399(4)	C(302)-C(303)	1.324(5)
C(10)-C(15)	1.389(4)	C(303)-C(304)	1.467(4)
C(10)-C(11)	1.543(4)	C(304)-C(309)	1.386(5)
C(11)-C(14)	1.535(5)	C(304)-C(305)	1.401(5)
C(11)-C(13)	1.535(5)	C(305)-C(306)	1.387(5)
C(11)-C(12)	1.536(5)	C(306)-C(307)	1.382(5)
C(16)-C(29)	1.404(3)	C(307)-C(308)	1.373(6)
C(16)-C(17)	1.420(4)	C(308)-C(309)	1.391(5)
C(17)-C(18)	1.437(4)		
Na(1B)-O(3B)#2	2.287(2)	C(18B)-C(23B)	1.402(4)
Na(1B)-O(1B)	2.322(2)	C(18B)-C(19B)	1.534(4)
Na(1B)-O(401)	2.335(3)	C(19B)-C(20B)	1.533(5)
Na(1B)-O(2B)	2.390(2)	C(19B)-C(21B)	1.535(4)
Na(1B)-C(17B)	2.691(3)	C(19B)-C(22B)	1.535(5)
Na(1B)-C(16B)	2.998(3)	C(23B)-C(24B)	1.391(4)
Na(1B)-C(3B)	3.117(3)	C(24B)-C(29B)	1.392(4)
Na(1B)-Na(2B)#2	3.1195(15)	C(24B)-C(25B)	1.543(4)
Na(1B)-Na(3B)#2	3.1196(15)	C(25B)-C(28B)	1.529(4)
Na(1B)-Na(2B)	4.1287(15)	C(25B)-C(26B)	1.532(5)
Na(1B)-Na(3B)	4.1655(15)	C(25B)-C(27B)	1.538(5)
Na(2B)-O(1B)#2	2.264(2)	C(30B)-C(43B)	1.399(4)
Na(2B)-O(501)	2.264(3)	C(30B)-C(31B)	1.430(3)
Na(2B)-O(2B)	2.292(2)	C(31B)-C(32B)	1.427(4)
Na(2B)-O(3B)	2.387(2)	C(32B)-C(37B)	1.390(4)
Na(2B)-C(31B)	2.717(3)	C(32B)-C(33B)	1.541(4)
Na(2B)-C(30B)	3.022(3)	C(33B)-C(36B)	1.533(5)
Na(2B)-Na(3B)#2	3.0864(15)	C(33B)-C(35B)	1.541(4)
Na(2B)-Na(1B)#2	3.1195(15)	C(33B)-C(34B)	1.541(5)
Na(2B)-C(17B)	3.127(3)	C(37B)-C(38B)	1.402(4)
Na(2B)-Na(3B)	4.1625(15)	C(38B)-C(43B)	1.389(4)
Na(3B)-O(2B)#2	2.277(2)	C(38B)-C(39B)	1.535(4)
Na(3B)-O(3B)	2.298(2)	C(39B)-C(41B)	1.527(5)
Na(3B)-O(601)	2.321(3)	C(39B)-C(42B)	1.538(5)
Na(3B)-O(1B)	2.367(2)	C(39B)-C(40B)	1.541(5)
Na(3B)-C(3B)	2.702(3)	O(401)-C(401)	1.226(5)
Na(3B)-C(2B)	3.033(3)	C(401)-C(402)	1.449(5)
Na(3B)-Na(2B)#2	3.0864(15)	C(402)-C(403)	1.332(5)
Na(3B)-C(31B)	3.114(3)	C(403)-C(404)	1.461(5)
Na(3B)-Na(1B)#2	3.1196(15)	C(404)-C(409)	1.371(5)
O(1B)-C(3B)	1.337(3)	C(404)-C(405)	1.375(5)
O(1B)-Na(2B)#2	2.264(2)	C(405)-C(406)	1.384(6)
O(2B)-C(17B)	1.339(3)	C(406)-C(407)	1.381(7)
O(2B)-Na(3B)#2	2.277(2)	C(407)-C(408)	1.346(6)
O(3B)-C(31B)	1.340(3)	C(408)-C(409)	1.393(6)
O(3B)-Na(1B)#2	2.287(2)	O(501)-C(501)	1.222(4)
C(1B)-C(30B)	1.536(3)	C(501)-C(502)	1.441(5)
C(1B)-C(16B)	1.539(3)	C(502)-C(503)	1.334(5)
C(1B)-C(2B)	1.540(3)	C(503)-C(504)	1.452(5)
C(2B)-C(15B)	1.391(4)	C(504)-C(505)	1.389(5)
C(2B)-C(3B)	1.427(4)	C(504)-C(509)	1.389(6)

C(3B)-C(4B)	1.439(4)	C(505)-C(506)	1.367(7)
C(4B)-C(9B)	1.400(4)	C(506)-C(507)	1.380(9)
C(4B)-C(5B)	1.536(4)	C(507)-C(508)	1.385(8)
C(5B)-C(8B)	1.542(5)	C(508)-C(509)	1.381(6)
C(5B)-C(7B)	1.542(4)	O(601)-C(601)	1.214(4)
C(5B)-C(6B)	1.545(5)	C(601)-C(602)	1.450(4)
C(9B)-C(10B)	1.391(4)	C(602)-C(603)	1.330(5)
C(10B)-C(15B)	1.391(4)	C(603)-C(604)	1.465(5)
C(10B)-C(11B)	1.540(4)	C(604)-C(605)	1.385(6)
C(11B)-C(13B)	1.531(4)	C(604)-C(609)	1.392(6)
C(11B)-C(14B)	1.534(4)	C(605)-C(606)	1.397(6)
C(11B)-C(12B)	1.540(5)	C(606)-C(607)	1.379(8)
C(16B)-C(29B)	1.397(3)	C(607)-C(608)	1.388(9)
C(16B)-C(17B)	1.429(4)	C(608)-C(609)	1.372(7)
C(17B)-C(18B)	1.434(4)		
O(91)-C(93A)	1.291(17)	C(91)-C(92)	1.374(9)
O(91)-C(91)	1.390(7)	C(93A)-C(94A)	1.214(16)
O(91)-C(93B)	1.428(10)	C(93B)-C(94B)	1.250(18)
O(3)#1-Na(1)-O(1)	96.10(7)	Na(1)-O(1)-Na(3)	123.56(8)
O(3)#1-Na(1)-O(101)	134.96(9)	C(17)-O(2)-Na(3)#1	156.55(17)
O(1)-Na(1)-O(101)	101.19(10)	C(17)-O(2)-Na(2)	116.06(16)
O(3)#1-Na(1)-O(2)	92.65(7)	Na(3)#1-O(2)-Na(2)	86.75(7)
O(1)-Na(1)-O(2)	111.04(8)	C(17)-O(2)-Na(1)	85.03(14)
O(101)-Na(1)-O(2)	118.42(9)	Na(3)#1-O(2)-Na(1)	84.78(7)
O(3)#1-Na(1)-C(17)	121.78(8)	Na(2)-O(2)-Na(1)	127.65(9)
O(1)-Na(1)-C(17)	111.37(8)	C(31)-O(3)-Na(1)#1	158.61(17)
O(101)-Na(1)-C(17)	89.75(9)	C(31)-O(3)-Na(3)	114.78(15)
O(2)-Na(1)-C(17)	30.17(7)	Na(1)#1-O(3)-Na(3)	86.47(7)
O(3)#1-Na(1)-C(16)	141.53(8)	C(31)-O(3)-Na(2)	86.97(14)
O(1)-Na(1)-C(16)	85.97(7)	Na(1)#1-O(3)-Na(2)	83.12(7)
O(101)-Na(1)-C(16)	81.36(8)	Na(3)-O(3)-Na(2)	122.51(8)
O(2)-Na(1)-C(16)	51.76(7)	C(16)-C(1)-C(30)	111.8(2)
C(17)-Na(1)-C(16)	28.77(7)	C(16)-C(1)-C(2)	112.6(2)
O(3)#1-Na(1)-Na(2)#1	50.06(5)	C(30)-C(1)-C(2)	112.5(2)
O(1)-Na(1)-Na(2)#1	46.27(5)	C(16)-C(1)-Na(3)	151.67(17)
O(101)-Na(1)-Na(2)#1	128.01(8)	C(30)-C(1)-Na(3)	91.92(14)
O(2)-Na(1)-Na(2)#1	111.86(6)	C(2)-C(1)-Na(3)	68.90(13)
C(17)-Na(1)-Na(2)#1	135.32(7)	C(15)-C(2)-C(3)	120.0(2)
C(16)-Na(1)-Na(2)#1	123.70(6)	C(15)-C(2)-C(1)	120.3(2)
O(3)#1-Na(1)-Na(3)#1	47.46(5)	C(3)-C(2)-C(1)	119.7(2)
O(1)-Na(1)-Na(3)#1	114.75(6)	C(15)-C(2)-Na(3)	124.37(18)
O(101)-Na(1)-Na(3)#1	143.86(9)	C(3)-C(2)-Na(3)	66.39(14)
O(2)-Na(1)-Na(3)#1	45.60(5)	C(1)-C(2)-Na(3)	81.35(13)
C(17)-Na(1)-Na(3)#1	74.34(6)	O(1)-C(3)-C(2)	119.3(2)
C(16)-Na(1)-Na(3)#1	96.97(6)	O(1)-C(3)-C(4)	122.3(2)
Na(2)#1-Na(1)-Na(3)#1	82.91(4)	C(2)-C(3)-C(4)	118.3(2)
O(3)#1-Na(1)-Na(3)	87.85(6)	O(1)-C(3)-Na(3)	65.45(13)
O(1)-Na(1)-Na(3)	29.05(5)	C(2)-C(3)-Na(3)	84.22(15)
O(101)-Na(1)-Na(3)	124.83(9)	C(4)-C(3)-Na(3)	119.14(18)
O(2)-Na(1)-Na(3)	83.71(5)	C(9)-C(4)-C(3)	118.2(3)
C(17)-Na(1)-Na(3)	92.76(6)	C(9)-C(4)-C(5)	120.4(3)
C(16)-Na(1)-Na(3)	75.52(6)	C(3)-C(4)-C(5)	121.4(2)
Na(2)#1-Na(1)-Na(3)	48.18(3)	C(8)-C(5)-C(7)	110.3(3)
Na(3)#1-Na(1)-Na(3)	88.82(3)	C(8)-C(5)-C(4)	109.7(3)
O(1)#1-Na(2)-O(2)	96.43(8)	C(7)-C(5)-C(4)	110.5(3)
O(1)#1-Na(2)-O(201)	128.24(10)	C(8)-C(5)-C(6)	107.0(3)
O(2)-Na(2)-O(201)	106.75(9)	C(7)-C(5)-C(6)	106.6(3)
O(1)#1-Na(2)-O(3)	94.65(7)	C(4)-C(5)-C(6)	112.7(3)
O(2)-Na(2)-O(3)	112.44(8)	C(4)-C(9)-C(10)	124.2(3)
O(201)-Na(2)-O(3)	116.59(9)	C(15)-C(10)-C(9)	116.8(3)
O(1)#1-Na(2)-C(31)	123.57(8)	C(15)-C(10)-C(11)	122.5(3)

O(2)-Na(2)-C(31)	111.70(8)	C(9)-C(10)-C(11)	120.7(3)
O(201)-Na(2)-C(31)	89.87(9)	C(14)-C(11)-C(13)	109.7(3)
O(3)-Na(2)-C(31)	29.91(7)	C(14)-C(11)-C(12)	108.2(3)
O(1)#1-Na(2)-C(30)	143.11(8)	C(13)-C(11)-C(12)	108.2(3)
O(2)-Na(2)-C(30)	86.09(7)	C(14)-C(11)-C(10)	109.7(3)
O(201)-Na(2)-C(30)	85.18(9)	C(13)-C(11)-C(10)	109.2(3)
O(3)-Na(2)-C(30)	51.49(7)	C(12)-C(11)-C(10)	111.8(3)
C(31)-Na(2)-C(30)	28.59(7)	C(10)-C(15)-C(2)	122.4(3)
O(1)#1-Na(2)-Na(1)#1	48.07(5)	C(29)-C(16)-C(17)	120.1(2)
O(2)-Na(2)-Na(1)#1	115.21(6)	C(29)-C(16)-C(1)	120.6(2)
O(201)-Na(2)-Na(1)#1	138.03(9)	C(17)-C(16)-C(1)	119.2(2)
O(3)-Na(2)-Na(1)#1	46.81(5)	C(29)-C(16)-Na(1)	124.81(17)
C(31)-Na(2)-Na(1)#1	75.55(6)	C(17)-C(16)-Na(1)	63.93(14)
C(30)-Na(2)-Na(1)#1	97.71(6)	C(1)-C(16)-Na(1)	83.72(14)
O(1)#1-Na(2)-C(201)	142.33(10)	O(2)-C(17)-C(16)	119.9(2)
O(2)-Na(2)-C(201)	89.66(9)	O(2)-C(17)-C(18)	122.1(2)
O(201)-Na(2)-C(201)	19.51(10)	C(16)-C(17)-C(18)	117.9(2)
O(3)-Na(2)-C(201)	117.23(9)	O(2)-C(17)-Na(1)	64.80(13)
C(31)-Na(2)-C(201)	87.51(9)	C(16)-C(17)-Na(1)	87.30(15)
C(30)-Na(2)-C(201)	74.24(9)	C(18)-C(17)-Na(1)	116.63(18)
Na(1)#1-Na(2)-C(201)	153.62(8)	O(2)-C(17)-Na(2)	41.35(12)
O(1)#1-Na(2)-C(17)	119.02(8)	C(16)-C(17)-Na(2)	94.62(15)
O(2)-Na(2)-C(17)	22.60(6)	C(18)-C(17)-Na(2)	135.01(18)
O(201)-Na(2)-C(17)	91.06(9)	Na(1)-C(17)-Na(2)	93.61(8)
O(3)-Na(2)-C(17)	107.41(7)	C(23)-C(18)-C(17)	119.0(3)
C(31)-Na(2)-C(17)	96.17(8)	C(23)-C(18)-C(19)	120.5(2)
C(30)-Na(2)-C(17)	68.11(7)	C(17)-C(18)-C(19)	120.5(2)
Na(1)#1-Na(2)-C(17)	129.00(6)	C(22)-C(19)-C(21)	107.1(3)
C(201)-Na(2)-C(17)	72.08(9)	C(22)-C(19)-C(20)	111.3(3)
O(1)#1-Na(2)-Na(3)#1	50.69(6)	C(21)-C(19)-C(20)	106.8(3)
O(2)-Na(2)-Na(3)#1	46.08(5)	C(22)-C(19)-C(18)	109.9(3)
O(201)-Na(2)-Na(3)#1	127.71(8)	C(21)-C(19)-C(18)	112.0(3)
O(3)-Na(2)-Na(3)#1	115.41(6)	C(20)-C(19)-C(18)	109.7(3)
C(31)-Na(2)-Na(3)#1	137.98(7)	C(18)-C(23)-C(24)	123.7(3)
C(30)-Na(2)-Na(3)#1	124.91(6)	C(29)-C(24)-C(23)	116.5(2)
Na(1)#1-Na(2)-Na(3)#1	84.40(4)	C(29)-C(24)-C(25)	123.0(3)
C(201)-Na(2)-Na(3)#1	121.05(8)	C(23)-C(24)-C(25)	120.4(3)
C(17)-Na(2)-Na(3)#1	68.59(6)	C(26)-C(25)-C(28)	108.5(3)
O(1)#1-Na(2)-Na(3)	87.60(6)	C(26)-C(25)-C(24)	111.8(3)
O(2)-Na(2)-Na(3)	86.10(6)	C(28)-C(25)-C(24)	110.7(3)
O(201)-Na(2)-Na(3)	138.41(8)	C(26)-C(25)-C(27)	108.2(3)
O(3)-Na(2)-Na(3)	28.31(5)	C(28)-C(25)-C(27)	109.1(3)
C(31)-Na(2)-Na(3)	49.20(6)	C(24)-C(25)-C(27)	108.4(3)
C(30)-Na(2)-Na(3)	55.76(5)	C(24)-C(29)-C(16)	122.8(3)
Na(1)#1-Na(2)-Na(3)	49.12(3)	C(43)-C(30)-C(31)	120.2(2)
C(201)-Na(2)-Na(3)	129.99(8)	C(43)-C(30)-C(1)	119.8(2)
C(17)-Na(2)-Na(3)	87.16(5)	C(31)-C(30)-C(1)	120.1(2)
Na(3)#1-Na(2)-Na(3)	89.93(3)	C(43)-C(30)-Na(2)	126.04(18)
O(2)#1-Na(3)-O(3)	95.25(7)	C(31)-C(30)-Na(2)	63.96(14)
O(2)#1-Na(3)-O(301)	132.29(9)	C(1)-C(30)-Na(2)	82.38(14)
O(3)-Na(3)-O(301)	97.30(8)	O(3)-C(31)-C(30)	119.8(2)
O(2)#1-Na(3)-O(1)	92.24(7)	O(3)-C(31)-C(32)	122.5(2)
O(3)-Na(3)-O(1)	115.10(7)	C(30)-C(31)-C(32)	117.7(2)
O(301)-Na(3)-O(1)	122.52(9)	O(3)-C(31)-Na(2)	63.12(13)
O(2)#1-Na(3)-C(3)	121.25(9)	C(30)-C(31)-Na(2)	87.45(15)
O(3)-Na(3)-C(3)	115.08(8)	C(32)-C(31)-Na(2)	118.84(18)
O(301)-Na(3)-C(3)	94.04(9)	O(3)-C(31)-Na(3)	42.42(11)
O(1)-Na(3)-C(3)	30.01(7)	C(30)-C(31)-Na(3)	91.78(15)
O(2)#1-Na(3)-C(2)	141.69(8)	C(32)-C(31)-Na(3)	137.50(18)
O(3)-Na(3)-C(2)	88.84(7)	Na(2)-C(31)-Na(3)	90.47(8)
O(301)-Na(3)-C(2)	84.50(8)	C(37)-C(32)-C(31)	118.9(2)
O(1)-Na(3)-C(2)	52.39(7)	C(37)-C(32)-C(33)	120.3(2)
C(3)-Na(3)-C(2)	29.38(8)	C(31)-C(32)-C(33)	120.8(2)

O(2)#1-Na(3)-C(1)	125.42(8)	C(35)-C(33)-C(36)	107.1(3)
O(3)-Na(3)-C(1)	62.46(7)	C(35)-C(33)-C(34)	107.1(3)
O(301)-Na(3)-C(1)	101.02(8)	C(36)-C(33)-C(34)	110.1(3)
O(1)-Na(3)-C(1)	61.25(7)	C(35)-C(33)-C(32)	112.7(2)
C(3)-Na(3)-C(1)	52.62(8)	C(36)-C(33)-C(32)	109.0(2)
C(2)-Na(3)-C(1)	29.75(7)	C(34)-C(33)-C(32)	110.7(2)
O(2)#1-Na(3)-C(31)	117.97(8)	C(32)-C(37)-C(38)	124.0(3)
O(3)-Na(3)-C(31)	22.80(6)	C(43)-C(38)-C(37)	116.5(2)
O(301)-Na(3)-C(31)	82.78(8)	C(43)-C(38)-C(39)	122.4(2)
O(1)-Na(3)-C(31)	109.40(7)	C(37)-C(38)-C(39)	121.1(2)
C(3)-Na(3)-C(31)	98.74(8)	C(38)-C(39)-C(42)	110.6(2)
C(2)-Na(3)-C(31)	70.01(7)	C(38)-C(39)-C(40)	112.5(2)
C(1)-Na(3)-C(31)	48.93(7)	C(42)-C(39)-C(40)	107.5(3)
O(2)#1-Na(3)-Na(2)#1	47.17(5)	C(38)-C(39)-C(41)	108.8(3)
O(3)-Na(3)-Na(2)#1	116.31(6)	C(42)-C(39)-C(41)	109.5(3)
O(301)-Na(3)-Na(2)#1	146.35(8)	C(40)-C(39)-C(41)	107.9(3)
O(1)-Na(3)-Na(2)#1	45.39(5)	C(38)-C(43)-C(30)	122.7(2)
C(3)-Na(3)-Na(2)#1	74.10(7)	C(101)-O(101)-Na(1)	123.9(2)
C(2)-Na(3)-Na(2)#1	97.30(6)	O(101)-C(101)-C(102)	124.5(4)
C(1)-Na(3)-Na(2)#1	96.37(6)	C(103)-C(102)-C(101)	121.3(3)
C(31)-Na(3)-Na(2)#1	129.54(6)	C(102)-C(103)-C(104)	127.2(3)
O(2)#1-Na(3)-Na(1)#1	49.62(5)	C(105)-C(104)-C(109)	116.9(4)
O(3)-Na(3)-Na(1)#1	46.07(5)	C(105)-C(104)-C(103)	122.1(4)
O(301)-Na(3)-Na(1)#1	120.95(8)	C(109)-C(104)-C(103)	120.9(4)
O(1)-Na(3)-Na(1)#1	115.60(6)	C(104)-C(105)-C(106)	120.5(4)
C(3)-Na(3)-Na(1)#1	139.35(7)	C(107)-C(106)-C(105)	121.0(5)
C(2)-Na(3)-Na(1)#1	127.13(7)	C(108)-C(107)-C(106)	118.7(5)
C(1)-Na(3)-Na(1)#1	97.39(6)	C(107)-C(108)-C(109)	121.3(5)
C(31)-Na(3)-Na(1)#1	68.86(6)	C(108)-C(109)-C(104)	121.6(5)
Na(2)#1-Na(3)-Na(1)#1	84.58(4)	C(201)-O(201)-Na(2)	120.7(2)
O(2)#1-Na(3)-Na(2)	86.12(6)	O(201)-C(201)-C(202)	124.4(4)
O(3)-Na(3)-Na(2)	29.18(5)	O(201)-C(201)-Na(2)	39.78(18)
O(301)-Na(3)-Na(2)	123.02(7)	C(202)-C(201)-Na(2)	163.9(3)
O(1)-Na(3)-Na(2)	87.87(5)	C(203)-C(202)-C(201)	120.6(3)
C(3)-Na(3)-Na(2)	97.03(7)	C(202)-C(203)-C(204)	127.9(3)
C(2)-Na(3)-Na(2)	79.16(6)	C(205)-C(204)-C(209)	118.3(3)
C(1)-Na(3)-Na(2)	49.42(5)	C(205)-C(204)-C(203)	119.0(3)
C(31)-Na(3)-Na(2)	40.33(5)	C(209)-C(204)-C(203)	122.7(3)
Na(2)#1-Na(3)-Na(2)	90.07(3)	C(206)-C(205)-C(204)	120.9(3)
Na(1)#1-Na(3)-Na(2)	47.97(3)	C(207)-C(206)-C(205)	120.1(3)
O(2)#1-Na(3)-Na(1)	84.95(6)	C(206)-C(207)-C(208)	120.0(3)
O(3)-Na(3)-Na(1)	89.50(6)	C(207)-C(208)-C(209)	120.3(3)
O(301)-Na(3)-Na(1)	140.78(7)	C(208)-C(209)-C(204)	120.4(3)
O(1)-Na(3)-Na(1)	27.39(5)	C(301)-O(301)-Na(3)	124.3(2)
C(3)-Na(3)-Na(1)	49.05(6)	O(301)-C(301)-C(302)	125.0(3)
C(2)-Na(3)-Na(1)	56.96(6)	C(303)-C(302)-C(301)	121.2(3)
C(1)-Na(3)-Na(1)	48.96(5)	C(302)-C(303)-C(304)	127.5(3)
C(31)-Na(3)-Na(1)	89.71(5)	C(309)-C(304)-C(305)	118.3(3)
Na(2)#1-Na(3)-Na(1)	47.42(3)	C(309)-C(304)-C(303)	119.5(3)
Na(1)#1-Na(3)-Na(1)	91.18(3)	C(305)-C(304)-C(303)	122.1(3)
Na(2)-Na(3)-Na(1)	61.10(3)	C(306)-C(305)-C(304)	120.4(3)
C(3)-O(1)-Na(2)#1	156.76(17)	C(307)-C(306)-C(305)	120.5(4)
C(3)-O(1)-Na(1)	117.48(16)	C(308)-C(307)-C(306)	119.7(3)
Na(2)#1-O(1)-Na(1)	85.66(7)	C(307)-C(308)-C(309)	120.4(3)
C(3)-O(1)-Na(3)	84.54(14)	C(304)-C(309)-C(308)	120.8(3)
Na(2)#1-O(1)-Na(3)	83.91(7)		
O(3B)#2-Na(1B)-O(1B)	95.46(7)	C(3B)-O(1B)-Na(2B)#2	159.26(17)
O(3B)#2-Na(1B)-O(401)	131.94(10)	C(3B)-O(1B)-Na(1B)	114.10(15)
O(1B)-Na(1B)-O(401)	99.73(10)	Na(2B)#2-O(1B)-Na(1B)	85.73(7)
O(3B)#2-Na(1B)-O(2B)	93.41(7)	C(3B)-O(1B)-Na(3B)	89.18(14)
O(1B)-Na(1B)-O(2B)	112.41(8)	Na(2B)#2-O(1B)-Na(3B)	83.56(7)
O(401)-Na(1B)-O(2B)	121.25(9)	Na(1B)-O(1B)-Na(3B)	125.34(9)

O(3B)#2-Na(1B)-C(17B)	122.29(8)	C(17B)-O(2B)-Na(3B)#2	158.05(17)
O(1B)-Na(1B)-C(17B)	112.37(8)	C(17B)-O(2B)-Na(2B)	116.40(16)
O(401)-Na(1B)-C(17B)	93.12(9)	Na(3B)#2-O(2B)-Na(2B)	84.99(7)
O(2B)-Na(1B)-C(17B)	29.82(7)	C(17B)-O(2B)-Na(1B)	87.61(14)
O(3B)#2-Na(1B)-C(16B)	141.74(8)	Na(3B)#2-O(2B)-Na(1B)	83.86(7)
O(1B)-Na(1B)-C(16B)	87.14(7)	Na(2B)-O(2B)-Na(1B)	123.69(9)
O(401)-Na(1B)-C(16B)	84.63(9)	C(31B)-O(3B)-Na(1B)#2	157.90(17)
O(2B)-Na(1B)-C(16B)	51.30(7)	C(31B)-O(3B)-Na(3B)	115.21(16)
C(17B)-Na(1B)-C(16B)	28.44(7)	Na(1B)#2-O(3B)-Na(3B)	85.75(7)
O(3B)#2-Na(1B)-C(3B)	118.51(8)	C(31B)-O(3B)-Na(2B)	89.02(14)
O(1B)-Na(1B)-C(3B)	23.05(6)	Na(1B)#2-O(3B)-Na(2B)	83.71(7)
O(401)-Na(1B)-C(3B)	83.68(9)	Na(3B)-O(3B)-Na(2B)	125.34(9)
O(2B)-Na(1B)-C(3B)	107.97(7)	C(30B)-C(1B)-C(16B)	113.2(2)
C(17B)-Na(1B)-C(3B)	97.01(8)	C(30B)-C(1B)-C(2B)	111.7(2)
C(16B)-Na(1B)-C(3B)	69.14(7)	C(16B)-C(1B)-C(2B)	112.2(2)
O(3B)#2-Na(1B)-Na(2B)#2	49.51(5)	C(15B)-C(2B)-C(3B)	119.9(2)
O(1B)-Na(1B)-Na(2B)#2	46.36(5)	C(15B)-C(2B)-C(1B)	120.5(2)
O(401)-Na(1B)-Na(2B)#2	123.19(9)	C(3B)-C(2B)-C(1B)	119.5(2)
O(2B)-Na(1B)-Na(2B)#2	114.47(6)	C(15B)-C(2B)-Na(3B)	128.35(17)
C(17B)-Na(1B)-Na(2B)#2	137.62(7)	C(3B)-C(2B)-Na(3B)	62.95(13)
C(16B)-Na(1B)-Na(2B)#2	125.71(6)	C(1B)-C(2B)-Na(3B)	81.46(13)
C(3B)-Na(1B)-Na(2B)#2	69.30(6)	O(1B)-C(3B)-C(2B)	120.0(2)
O(3B)#2-Na(1B)-Na(3B)#2	47.28(5)	O(1B)-C(3B)-C(4B)	122.4(2)
O(1B)-Na(1B)-Na(3B)#2	115.16(6)	C(2B)-C(3B)-C(4B)	117.6(2)
O(401)-Na(1B)-Na(3B)#2	145.10(9)	O(1B)-C(3B)-Na(3B)	61.16(12)
O(2B)-Na(1B)-Na(3B)#2	46.52(5)	C(2B)-C(3B)-Na(3B)	88.98(15)
C(17B)-Na(1B)-Na(3B)#2	75.01(6)	C(4B)-C(3B)-Na(3B)	119.41(17)
C(16B)-Na(1B)-Na(3B)#2	97.36(6)	O(1B)-C(3B)-Na(1B)	42.85(12)
C(3B)-Na(1B)-Na(3B)#2	129.71(6)	C(2B)-C(3B)-Na(1B)	93.57(15)
Na(2B)#2-Na(1B)-Na(3B)#2	83.69(4)	C(4B)-C(3B)-Na(1B)	134.75(18)
O(3B)#2-Na(1B)-Na(2B)	85.33(6)	Na(3B)-C(3B)-Na(1B)	91.15(8)
O(1B)-Na(1B)-Na(2B)	87.07(6)	C(9B)-C(4B)-C(3B)	119.0(2)
O(401)-Na(1B)-Na(2B)	140.44(8)	C(9B)-C(4B)-C(5B)	119.8(2)
O(2B)-Na(1B)-Na(2B)	27.52(5)	C(3B)-C(4B)-C(5B)	121.2(2)
C(17B)-Na(1B)-Na(2B)	49.23(6)	C(4B)-C(5B)-C(8B)	108.3(3)
C(16B)-Na(1B)-Na(2B)	56.62(5)	C(4B)-C(5B)-C(7B)	112.6(3)
C(3B)-Na(1B)-Na(2B)	88.96(5)	C(8B)-C(5B)-C(7B)	107.8(3)
Na(2B)#2-Na(1B)-Na(2B)	89.49(4)	C(4B)-C(5B)-C(6B)	111.7(2)
Na(3B)#2-Na(1B)-Na(2B)	47.95(3)	C(8B)-C(5B)-C(6B)	110.4(3)
O(3B)#2-Na(1B)-Na(3B)	86.62(6)	C(7B)-C(5B)-C(6B)	105.9(3)
O(1B)-Na(1B)-Na(3B)	27.62(5)	C(10B)-C(9B)-C(4B)	123.6(2)
O(401)-Na(1B)-Na(3B)	124.05(9)	C(9B)-C(10B)-C(15B)	116.6(2)
O(2B)-Na(1B)-Na(3B)	86.93(5)	C(9B)-C(10B)-C(11B)	123.8(2)
C(17B)-Na(1B)-Na(3B)	95.72(6)	C(15B)-C(10B)-C(11B)	119.6(3)
C(16B)-Na(1B)-Na(3B)	78.22(5)	C(13B)-C(11B)-C(14B)	108.1(3)
C(3B)-Na(1B)-Na(3B)	40.43(5)	C(13B)-C(11B)-C(12B)	108.5(3)
Na(2B)#2-Na(1B)-Na(3B)	47.50(3)	C(14B)-C(11B)-C(12B)	108.8(3)
Na(3B)#2-Na(1B)-Na(3B)	90.16(3)	C(13B)-C(11B)-C(10B)	112.5(3)
Na(2B)-Na(1B)-Na(3B)	60.24(3)	C(14B)-C(11B)-C(10B)	109.6(2)
O(1B)#2-Na(2B)-O(501)	133.25(9)	C(12B)-C(11B)-C(10B)	109.3(2)
O(1B)#2-Na(2B)-O(2B)	96.61(8)	C(2B)-C(15B)-C(10B)	123.3(3)
O(501)-Na(2B)-O(2B)	112.53(9)	C(29B)-C(16B)-C(17B)	119.6(2)
O(1B)#2-Na(2B)-O(3B)	94.28(7)	C(29B)-C(16B)-C(1B)	120.9(2)
O(501)-Na(2B)-O(3B)	106.09(9)	C(17B)-C(16B)-C(1B)	119.5(2)
O(2B)-Na(2B)-O(3B)	112.68(8)	C(29B)-C(16B)-Na(1B)	125.62(17)
O(1B)#2-Na(2B)-C(31B)	122.81(8)	C(17B)-C(16B)-Na(1B)	63.73(14)
O(501)-Na(2B)-C(31B)	79.92(9)	C(1B)-C(16B)-Na(1B)	80.88(14)
O(2B)-Na(2B)-C(31B)	112.04(8)	O(2B)-C(17B)-C(16B)	119.9(2)
O(3B)-Na(2B)-C(31B)	29.53(7)	O(2B)-C(17B)-C(18B)	122.1(2)
O(1B)#2-Na(2B)-C(30B)	142.53(8)	C(16B)-C(17B)-C(18B)	118.0(2)
O(501)-Na(2B)-C(30B)	77.24(8)	O(2B)-C(17B)-Na(1B)	62.57(13)
O(2B)-Na(2B)-C(30B)	86.89(7)	C(16B)-C(17B)-Na(1B)	87.83(15)
O(3B)-Na(2B)-C(30B)	50.98(7)	C(18B)-C(17B)-Na(1B)	118.91(18)

C(31B)-Na(2B)-C(30B)	28.22(7)	O(2B)-C(17B)-Na(2B)	41.05(11)
O(1B)#2-Na(2B)-Na(3B)#2	49.65(6)	C(16B)-C(17B)-Na(2B)	93.83(15)
O(501)-Na(2B)-Na(3B)#2	138.65(8)	C(18B)-C(17B)-Na(2B)	135.84(18)
O(2B)-Na(2B)-Na(3B)#2	47.29(5)	Na(1B)-C(17B)-Na(2B)	90.10(8)
O(3B)-Na(2B)-Na(3B)#2	115.03(6)	C(23B)-C(18B)-C(17B)	118.8(2)
C(31B)-Na(2B)-Na(3B)#2	137.96(7)	C(23B)-C(18B)-C(19B)	120.1(2)
C(30B)-Na(2B)-Na(3B)#2	126.25(6)	C(17B)-C(18B)-C(19B)	121.1(2)
O(1B)#2-Na(2B)-Na(1B)#2	47.92(6)	C(20B)-C(19B)-C(18B)	109.6(3)
O(501)-Na(2B)-Na(1B)#2	130.17(8)	C(20B)-C(19B)-C(21B)	106.9(3)
O(2B)-Na(2B)-Na(1B)#2	116.62(6)	C(18B)-C(19B)-C(21B)	112.9(3)
O(3B)-Na(2B)-Na(1B)#2	46.77(5)	C(20B)-C(19B)-C(22B)	110.3(3)
C(31B)-Na(2B)-Na(1B)#2	74.91(6)	C(18B)-C(19B)-C(22B)	110.4(3)
C(30B)-Na(2B)-Na(1B)#2	97.38(6)	C(21B)-C(19B)-C(22B)	106.5(3)
Na(3B)#2-Na(2B)-Na(1B)#2	84.32(4)	C(24B)-C(23B)-C(18B)	123.8(2)
O(1B)#2-Na(2B)-C(17B)	119.16(8)	C(23B)-C(24B)-C(29B)	116.5(2)
O(501)-Na(2B)-C(17B)	94.40(9)	C(23B)-C(24B)-C(25B)	123.4(2)
O(2B)-Na(2B)-C(17B)	22.56(7)	C(29B)-C(24B)-C(25B)	120.0(2)
O(3B)-Na(2B)-C(17B)	107.63(7)	C(28B)-C(25B)-C(26B)	108.0(3)
C(31B)-Na(2B)-C(17B)	96.61(8)	C(28B)-C(25B)-C(27B)	107.9(3)
C(30B)-Na(2B)-C(17B)	68.97(7)	C(26B)-C(25B)-C(27B)	109.3(3)
Na(3B)#2-Na(2B)-C(17B)	69.78(6)	C(28B)-C(25B)-C(24B)	112.2(3)
Na(1B)#2-Na(2B)-C(17B)	130.36(6)	C(26B)-C(25B)-C(24B)	110.2(3)
O(1B)#2-Na(2B)-Na(1B)	87.70(6)	C(27B)-C(25B)-C(24B)	109.2(3)
O(501)-Na(2B)-Na(1B)	134.27(8)	C(24B)-C(29B)-C(16B)	123.2(2)
O(2B)-Na(2B)-Na(1B)	28.80(5)	C(43B)-C(30B)-C(31B)	119.8(2)
O(3B)-Na(2B)-Na(1B)	86.20(5)	C(43B)-C(30B)-C(1B)	120.9(2)
C(31B)-Na(2B)-Na(1B)	94.76(6)	C(31B)-C(30B)-C(1B)	119.3(2)
C(30B)-Na(2B)-Na(1B)	77.61(6)	C(43B)-C(30B)-Na(2B)	128.76(18)
Na(3B)#2-Na(2B)-Na(1B)	48.64(3)	C(31B)-C(30B)-Na(2B)	63.96(14)
Na(1B)#2-Na(2B)-Na(1B)	90.51(4)	C(1B)-C(30B)-Na(2B)	80.40(13)
C(17B)-Na(2B)-Na(1B)	40.67(5)	O(3B)-C(31B)-C(32B)	122.1(2)
O(1B)#2-Na(2B)-Na(3B)	86.45(6)	O(3B)-C(31B)-C(30B)	119.9(2)
O(501)-Na(2B)-Na(3B)	128.25(7)	C(32B)-C(31B)-C(30B)	118.0(2)
O(2B)-Na(2B)-Na(3B)	88.25(6)	O(3B)-C(31B)-Na(2B)	61.45(13)
O(3B)-Na(2B)-Na(3B)	26.77(5)	C(32B)-C(31B)-Na(2B)	119.68(18)
C(31B)-Na(2B)-Na(3B)	48.43(6)	C(30B)-C(31B)-Na(2B)	87.82(15)
C(30B)-Na(2B)-Na(3B)	56.29(5)	O(3B)-C(31B)-Na(3B)	41.89(12)
Na(3B)#2-Na(2B)-Na(3B)	90.68(4)	C(32B)-C(31B)-Na(3B)	134.03(18)
Na(1B)#2-Na(2B)-Na(3B)	48.15(3)	C(30B)-C(31B)-Na(3B)	94.85(16)
C(17B)-Na(2B)-Na(3B)	89.39(6)	Na(2B)-C(31B)-Na(3B)	90.83(8)
Na(1B)-Na(2B)-Na(3B)	60.32(3)	C(37B)-C(32B)-C(31B)	118.9(2)
O(2B)#2-Na(3B)-O(3B)	96.19(7)	C(37B)-C(32B)-C(33B)	119.9(3)
O(2B)#2-Na(3B)-O(601)	129.55(9)	C(31B)-C(32B)-C(33B)	121.2(2)
O(3B)-Na(3B)-O(601)	102.56(9)	C(36B)-C(33B)-C(32B)	109.9(2)
O(2B)#2-Na(3B)-O(1B)	94.19(7)	C(36B)-C(33B)-C(35B)	106.5(3)
O(3B)-Na(3B)-O(1B)	111.30(8)	C(32B)-C(33B)-C(35B)	112.4(3)
O(601)-Na(3B)-O(1B)	120.51(9)	C(36B)-C(33B)-C(34B)	110.9(3)
O(2B)#2-Na(3B)-C(3B)	122.93(8)	C(32B)-C(33B)-C(34B)	109.7(3)
O(3B)-Na(3B)-C(3B)	110.87(8)	C(35B)-C(33B)-C(34B)	107.4(3)
O(601)-Na(3B)-C(3B)	93.14(9)	C(32B)-C(37B)-C(38B)	123.9(3)
O(1B)-Na(3B)-C(3B)	29.66(7)	C(43B)-C(38B)-C(37B)	116.3(2)
O(2B)#2-Na(3B)-C(2B)	142.05(8)	C(43B)-C(38B)-C(39B)	123.7(3)
O(3B)-Na(3B)-C(2B)	85.95(7)	C(37B)-C(38B)-C(39B)	120.0(3)
O(601)-Na(3B)-C(2B)	86.19(8)	C(41B)-C(39B)-C(38B)	112.1(2)
O(1B)-Na(3B)-C(2B)	50.84(7)	C(41B)-C(39B)-C(42B)	107.9(3)
C(3B)-Na(3B)-C(2B)	28.07(7)	C(38B)-C(39B)-C(42B)	111.0(3)
O(2B)#2-Na(3B)-Na(2B)#2	47.72(5)	C(41B)-C(39B)-C(40B)	108.5(3)
O(3B)-Na(3B)-Na(2B)#2	114.70(6)	C(38B)-C(39B)-C(40B)	108.5(3)
O(601)-Na(3B)-Na(2B)#2	142.72(9)	C(42B)-C(39B)-C(40B)	108.8(3)
O(1B)-Na(3B)-Na(2B)#2	46.79(5)	C(38B)-C(43B)-C(30B)	122.8(2)
C(3B)-Na(3B)-Na(2B)#2	75.23(6)	C(401)-O(401)-Na(1B)	121.1(2)
C(2B)-Na(3B)-Na(2B)#2	97.12(6)	O(401)-C(401)-C(402)	125.0(4)
O(2B)#2-Na(3B)-C(31B)	119.09(8)	C(403)-C(402)-C(401)	120.5(3)

O(3B)-Na(3B)-C(31B)	22.90(6)	C(402)-C(403)-C(404)	127.9(3)
O(601)-Na(3B)-C(31B)	86.59(9)	C(409)-C(404)-C(405)	116.7(4)
O(1B)-Na(3B)-C(31B)	107.02(7)	C(409)-C(404)-C(403)	123.0(3)
C(3B)-Na(3B)-C(31B)	95.85(8)	C(405)-C(404)-C(403)	120.2(4)
C(2B)-Na(3B)-C(31B)	68.32(7)	C(404)-C(405)-C(406)	121.5(4)
Na(2B)#2-Na(3B)-C(31B)	129.20(6)	C(407)-C(406)-C(405)	120.6(4)
O(2B)#2-Na(3B)-Na(1B)#2	49.62(5)	C(408)-C(407)-C(406)	118.5(4)
O(3B)-Na(3B)-Na(1B)#2	46.97(5)	C(407)-C(408)-C(409)	120.6(5)
O(601)-Na(3B)-Na(1B)#2	124.51(8)	C(404)-C(409)-C(408)	122.0(4)
O(1B)-Na(3B)-Na(1B)#2	114.33(6)	C(501)-O(501)-Na(2B)	145.5(2)
C(3B)-Na(3B)-Na(1B)#2	137.10(7)	O(501)-C(501)-C(502)	125.2(4)
C(2B)-Na(3B)-Na(1B)#2	125.20(6)	C(503)-C(502)-C(501)	120.8(4)
Na(2B)#2-Na(3B)-Na(1B)#2	83.40(4)	C(502)-C(503)-C(504)	127.7(4)
C(31B)-Na(3B)-Na(1B)#2	69.73(5)	C(505)-C(504)-C(509)	118.0(4)
O(2B)#2-Na(3B)-Na(2B)	87.32(6)	C(505)-C(504)-C(503)	120.7(4)
O(3B)-Na(3B)-Na(2B)	27.89(5)	C(509)-C(504)-C(503)	121.4(4)
O(601)-Na(3B)-Na(2B)	127.29(8)	C(506)-C(505)-C(504)	121.9(5)
O(1B)-Na(3B)-Na(2B)	85.71(5)	C(505)-C(506)-C(507)	119.3(5)
C(3B)-Na(3B)-Na(2B)	94.25(6)	C(506)-C(507)-C(508)	120.5(5)
C(2B)-Na(3B)-Na(2B)	77.05(5)	C(509)-C(508)-C(507)	119.4(6)
Na(2B)#2-Na(3B)-Na(2B)	89.32(4)	C(508)-C(509)-C(504)	121.0(5)
C(31B)-Na(3B)-Na(2B)	40.74(5)	C(601)-O(601)-Na(3B)	124.9(2)
Na(1B)#2-Na(3B)-Na(2B)	48.15(3)	O(601)-C(601)-C(602)	124.7(4)
O(2B)#2-Na(3B)-Na(1B)	86.55(6)	C(603)-C(602)-C(601)	121.5(4)
O(3B)-Na(3B)-Na(1B)	86.42(6)	C(602)-C(603)-C(604)	127.9(4)
O(601)-Na(3B)-Na(1B)	140.41(7)	C(605)-C(604)-C(609)	119.7(4)
O(1B)-Na(3B)-Na(1B)	27.05(5)	C(605)-C(604)-C(603)	122.0(4)
C(3B)-Na(3B)-Na(1B)	48.42(6)	C(609)-C(604)-C(603)	118.3(4)
C(2B)-Na(3B)-Na(1B)	55.68(5)	C(604)-C(605)-C(606)	120.0(5)
Na(2B)#2-Na(3B)-Na(1B)	48.18(3)	C(607)-C(606)-C(605)	119.8(6)
C(31B)-Na(3B)-Na(1B)	88.32(5)	C(606)-C(607)-C(608)	119.9(5)
Na(1B)#2-Na(3B)-Na(1B)	89.84(3)	C(609)-C(608)-C(607)	120.5(6)
Na(2B)-Na(3B)-Na(1B)	59.44(3)	C(608)-C(609)-C(604)	120.1(6)
C(93A)-O(91)-C(91)	119.5(10)	C(92)-C(91)-O(91)	113.5(6)
C(93A)-O(91)-C(93B)	32.8(9)	C(94A)-C(93A)-O(91)	120.8(18)
C(91)-O(91)-C(93B)	111.8(7)	C(94B)-C(93B)-O(91)	114.3(14)

Symmetry transformations used to generate equivalent atoms:
 #1 -x+1,-y,-z+2 #2 -x+2,-y+1,-z+1

Table 31. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a·6C₆H₅O** (trans-Cinnamaldehyde). The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Na(1)	29(1)	24(1)	31(1)	-9(1)	4(1)	-13(1)
Na(2)	31(1)	23(1)	29(1)	-9(1)	3(1)	-11(1)
Na(3)	30(1)	26(1)	28(1)	-11(1)	5(1)	-15(1)
O(1)	25(1)	24(1)	30(1)	-12(1)	3(1)	-11(1)
O(2)	31(1)	21(1)	25(1)	-6(1)	1(1)	-14(1)
O(3)	27(1)	21(1)	28(1)	-10(1)	6(1)	-12(1)
C(1)	21(1)	18(1)	24(1)	-9(1)	6(1)	-11(1)
C(2)	23(1)	23(1)	21(1)	-4(1)	2(1)	-12(1)
C(3)	24(1)	24(1)	26(1)	-7(1)	4(1)	-12(1)
C(4)	24(1)	29(1)	31(2)	-8(1)	3(1)	-12(1)
C(5)	24(1)	37(2)	40(2)	-13(1)	-1(1)	-9(1)

C(6)	25(2)	59(2)	76(3)	-30(2)	-4(2)	-9(2)
C(7)	31(2)	51(2)	52(2)	-20(2)	11(2)	-9(2)
C(8)	38(2)	34(2)	47(2)	-9(2)	-6(2)	-6(1)
C(9)	27(1)	38(2)	37(2)	-9(1)	-1(1)	-19(1)
C(10)	32(2)	32(2)	32(2)	-11(1)	1(1)	-19(1)
C(11)	41(2)	40(2)	38(2)	-17(1)	-2(1)	-24(2)
C(12)	58(2)	45(2)	52(2)	-27(2)	-1(2)	-25(2)
C(13)	68(3)	65(3)	71(3)	-30(2)	12(2)	-51(2)
C(14)	56(2)	57(2)	46(2)	-20(2)	-8(2)	-23(2)
C(15)	31(1)	27(1)	27(1)	-11(1)	3(1)	-15(1)
C(16)	21(1)	22(1)	24(1)	-7(1)	5(1)	-11(1)
C(17)	23(1)	19(1)	24(1)	-6(1)	3(1)	-9(1)
C(18)	32(2)	22(1)	27(1)	-4(1)	1(1)	-8(1)
C(19)	49(2)	31(2)	25(2)	-2(1)	-6(1)	-17(1)
C(20)	73(3)	40(2)	28(2)	-11(1)	3(2)	-27(2)
C(21)	86(3)	45(2)	33(2)	5(2)	-17(2)	-31(2)
C(22)	48(2)	52(2)	41(2)	-7(2)	-13(2)	-22(2)
C(23)	43(2)	24(1)	29(2)	-1(1)	3(1)	-15(1)
C(24)	37(2)	21(1)	37(2)	-9(1)	10(1)	-16(1)
C(25)	56(2)	28(2)	47(2)	-11(1)	14(2)	-28(2)
C(26)	83(3)	50(2)	61(2)	-19(2)	15(2)	-52(2)
C(27)	71(3)	27(2)	91(3)	-17(2)	22(2)	-23(2)
C(28)	86(3)	49(2)	55(2)	-12(2)	27(2)	-49(2)
C(29)	29(1)	24(1)	29(1)	-10(1)	7(1)	-14(1)
C(30)	23(1)	21(1)	21(1)	-8(1)	3(1)	-10(1)
C(31)	24(1)	21(1)	23(1)	-8(1)	3(1)	-9(1)
C(32)	26(1)	27(1)	27(1)	-10(1)	8(1)	-14(1)
C(33)	38(2)	32(2)	38(2)	-11(1)	17(1)	-21(1)
C(34)	48(2)	40(2)	40(2)	-5(2)	16(2)	-22(2)
C(35)	55(2)	45(2)	52(2)	-20(2)	34(2)	-29(2)
C(36)	38(2)	46(2)	60(2)	-23(2)	19(2)	-26(2)
C(37)	31(1)	33(2)	29(1)	-15(1)	12(1)	-16(1)
C(38)	34(2)	28(1)	32(2)	-15(1)	11(1)	-16(1)
C(39)	38(2)	28(2)	44(2)	-20(1)	18(1)	-17(1)
C(40)	76(3)	35(2)	85(3)	-31(2)	45(2)	-34(2)
C(41)	48(2)	51(2)	65(2)	-38(2)	11(2)	-22(2)
C(42)	45(2)	31(2)	45(2)	-17(1)	13(2)	-12(1)
C(43)	31(1)	22(1)	30(1)	-10(1)	9(1)	-15(1)
O(101)	53(2)	44(1)	73(2)	-18(1)	27(1)	-28(1)
C(101)	45(2)	40(2)	55(2)	-6(2)	21(2)	-18(2)
C(102)	51(2)	37(2)	46(2)	-10(2)	19(2)	-19(2)
C(103)	53(2)	48(2)	42(2)	-10(2)	14(2)	-21(2)
C(104)	55(2)	44(2)	51(2)	-14(2)	13(2)	-24(2)
C(105)	116(4)	93(4)	56(3)	-20(2)	18(3)	-81(3)
C(106)	133(5)	112(4)	76(3)	-22(3)	31(3)	-98(4)
C(107)	66(3)	65(3)	96(4)	-20(3)	11(3)	-41(2)
C(108)	100(4)	137(5)	87(4)	-30(4)	6(3)	-84(4)
C(109)	100(4)	126(5)	57(3)	-26(3)	9(3)	-75(4)
O(201)	50(2)	35(1)	61(2)	-19(1)	-4(1)	-5(1)
C(201)	43(2)	41(2)	50(2)	-18(2)	2(2)	-8(2)
C(202)	39(2)	37(2)	51(2)	-15(2)	2(2)	-7(2)
C(203)	36(2)	43(2)	51(2)	-13(2)	3(2)	-11(2)
C(204)	37(2)	37(2)	41(2)	-8(1)	1(1)	-12(1)
C(205)	35(2)	46(2)	50(2)	-8(2)	2(2)	-19(2)
C(206)	49(2)	41(2)	56(2)	-4(2)	-1(2)	-23(2)
C(207)	44(2)	34(2)	62(2)	-8(2)	-2(2)	-11(2)
C(208)	38(2)	40(2)	74(3)	-13(2)	4(2)	-14(2)
C(209)	40(2)	36(2)	69(2)	-10(2)	4(2)	-17(2)
O(301)	52(1)	54(2)	36(1)	-20(1)	3(1)	-23(1)
C(301)	41(2)	53(2)	35(2)	-16(2)	1(1)	-25(2)
C(302)	40(2)	50(2)	31(2)	-14(1)	0(1)	-15(2)
C(303)	35(2)	46(2)	34(2)	-10(1)	1(1)	-18(2)
C(304)	34(2)	50(2)	38(2)	-18(2)	8(1)	-20(2)

C(305)	35(2)	67(2)	49(2)	-28(2)	3(2)	-14(2)
C(306)	46(2)	83(3)	50(2)	-33(2)	-6(2)	-16(2)
C(307)	58(2)	80(3)	47(2)	-37(2)	14(2)	-31(2)
C(308)	50(2)	56(2)	55(2)	-33(2)	17(2)	-19(2)
C(309)	38(2)	47(2)	49(2)	-19(2)	5(2)	-13(2)
Na(1B)	31(1)	26(1)	29(1)	-7(1)	4(1)	-14(1)
Na(2B)	29(1)	27(1)	33(1)	-12(1)	6(1)	-13(1)
Na(3B)	29(1)	24(1)	32(1)	-10(1)	6(1)	-11(1)
O(1B)	31(1)	21(1)	27(1)	-7(1)	1(1)	-12(1)
O(2B)	24(1)	21(1)	32(1)	-9(1)	5(1)	-10(1)
O(3B)	27(1)	26(1)	27(1)	-12(1)	7(1)	-15(1)
C(1B)	17(1)	18(1)	22(1)	-7(1)	2(1)	-8(1)
C(2B)	18(1)	22(1)	24(1)	-4(1)	3(1)	-9(1)
C(3B)	22(1)	25(1)	21(1)	-6(1)	4(1)	-12(1)
C(4B)	25(1)	26(1)	25(1)	-3(1)	0(1)	-10(1)
C(5B)	38(2)	35(2)	28(2)	-6(1)	-5(1)	-12(1)
C(6B)	51(2)	45(2)	28(2)	-10(1)	-1(1)	-19(2)
C(7B)	62(2)	42(2)	37(2)	-4(2)	-16(2)	-8(2)
C(8B)	44(2)	66(2)	43(2)	-17(2)	-5(2)	-29(2)
C(9B)	27(1)	21(1)	31(2)	1(1)	-1(1)	-7(1)
C(10B)	23(1)	20(1)	32(1)	-3(1)	2(1)	-9(1)
C(11B)	37(2)	19(1)	41(2)	-5(1)	5(1)	-10(1)
C(12B)	92(3)	25(2)	61(2)	-15(2)	31(2)	-13(2)
C(13B)	37(2)	21(1)	61(2)	0(1)	-5(2)	-11(1)
C(14B)	50(2)	29(2)	61(2)	-5(2)	-12(2)	-20(2)
C(15B)	23(1)	22(1)	27(1)	-7(1)	5(1)	-11(1)
C(16B)	19(1)	21(1)	22(1)	-8(1)	4(1)	-7(1)
C(17B)	22(1)	24(1)	22(1)	-6(1)	3(1)	-11(1)
C(18B)	21(1)	26(1)	31(1)	-12(1)	4(1)	-7(1)
C(19B)	19(1)	30(2)	56(2)	-18(1)	6(1)	-6(1)
C(20B)	41(2)	45(2)	70(3)	-35(2)	20(2)	-14(2)
C(21B)	21(2)	40(2)	91(3)	-23(2)	11(2)	-6(1)
C(22B)	33(2)	29(2)	65(2)	-3(2)	-3(2)	-3(1)
C(23B)	20(1)	32(2)	39(2)	-12(1)	7(1)	-13(1)
C(24B)	23(1)	27(1)	35(2)	-8(1)	5(1)	-13(1)
C(25B)	25(1)	31(2)	54(2)	-10(1)	8(1)	-17(1)
C(26B)	41(2)	47(2)	74(3)	7(2)	3(2)	-25(2)
C(27B)	46(2)	41(2)	81(3)	-26(2)	15(2)	-28(2)
C(28B)	31(2)	45(2)	79(3)	-14(2)	13(2)	-25(2)
C(29B)	22(1)	20(1)	29(1)	-7(1)	5(1)	-7(1)
C(30B)	20(1)	20(1)	23(1)	-6(1)	3(1)	-7(1)
C(31B)	23(1)	20(1)	25(1)	-8(1)	6(1)	-10(1)
C(32B)	32(2)	28(1)	29(1)	-11(1)	9(1)	-16(1)
C(33B)	45(2)	47(2)	35(2)	-21(1)	23(1)	-30(2)
C(34B)	40(2)	54(2)	61(2)	-21(2)	24(2)	-29(2)
C(35B)	88(3)	87(3)	51(2)	-42(2)	51(2)	-66(3)
C(36B)	56(2)	46(2)	36(2)	-6(2)	14(2)	-33(2)
C(37B)	42(2)	36(2)	29(2)	-18(1)	14(1)	-20(1)
C(38B)	36(2)	28(1)	30(2)	-13(1)	6(1)	-17(1)
C(39B)	50(2)	36(2)	33(2)	-18(1)	8(1)	-25(2)
C(40B)	64(2)	48(2)	69(3)	-38(2)	18(2)	-26(2)
C(41B)	61(2)	45(2)	47(2)	-22(2)	10(2)	-38(2)
C(42B)	89(3)	66(2)	36(2)	-24(2)	10(2)	-52(2)
C(43B)	27(1)	21(1)	26(1)	-7(1)	6(1)	-12(1)
O(401)	87(2)	65(2)	47(2)	-13(1)	23(1)	-54(2)
C(401)	59(2)	68(3)	41(2)	-16(2)	18(2)	-45(2)
C(402)	73(3)	57(2)	50(2)	-24(2)	37(2)	-44(2)
C(403)	45(2)	61(2)	48(2)	-26(2)	21(2)	-31(2)
C(404)	42(2)	45(2)	56(2)	-21(2)	13(2)	-25(2)
C(405)	73(3)	63(3)	58(3)	-31(2)	13(2)	-10(2)
C(406)	99(4)	45(2)	70(3)	-17(2)	-6(3)	-14(2)
C(407)	75(3)	45(2)	77(3)	-10(2)	11(2)	-36(2)
C(408)	127(5)	44(3)	119(5)	-15(3)	82(4)	-31(3)

C(409)	128(4)	39(2)	112(4)	-21(2)	89(4)	-31(3)
O(501)	58(2)	44(1)	48(1)	-11(1)	-16(1)	-23(1)
C(501)	51(2)	37(2)	41(2)	-8(2)	-12(2)	-12(2)
C(502)	50(2)	35(2)	41(2)	-8(1)	-12(2)	-13(2)
C(503)	56(2)	37(2)	46(2)	-10(2)	-9(2)	-16(2)
C(504)	61(2)	44(2)	44(2)	-7(2)	-11(2)	-25(2)
C(505)	105(4)	91(4)	82(3)	-38(3)	8(3)	-67(3)
C(506)	124(5)	121(5)	108(5)	-45(4)	14(4)	-92(5)
C(507)	98(4)	111(5)	95(4)	5(4)	-12(3)	-76(4)
C(508)	68(3)	92(4)	72(3)	-3(3)	-5(3)	-35(3)
C(509)	60(3)	59(3)	63(3)	-12(2)	-6(2)	-25(2)
O(601)	52(2)	36(1)	76(2)	-25(1)	23(1)	-17(1)
C(601)	37(2)	30(2)	62(2)	-10(2)	15(2)	-9(1)
C(602)	36(2)	32(2)	61(2)	-15(2)	13(2)	-12(1)
C(603)	44(2)	37(2)	55(2)	-12(2)	13(2)	-18(2)
C(604)	65(2)	33(2)	43(2)	-9(2)	15(2)	-18(2)
C(605)	64(3)	51(2)	68(3)	-26(2)	23(2)	-13(2)
C(606)	90(4)	61(3)	76(3)	-21(3)	29(3)	-1(3)
C(607)	157(6)	37(2)	54(3)	-14(2)	28(3)	-1(3)
C(608)	168(7)	54(3)	65(3)	-27(3)	15(4)	-36(4)
C(609)	100(4)	51(2)	65(3)	-23(2)	13(3)	-32(3)
O(91)	28(2)	26(2)	40(3)	-11(2)	3(2)	-21(2)
C(91)	29(3)	44(4)	44(4)	9(3)	-2(3)	-13(3)
C(92)	42(4)	25(3)	96(6)	-11(4)	33(4)	-20(3)
C(93A)	90(20)	220(40)	26(11)	39(17)	62(14)	70(20)
C(93B)	27(7)	36(8)	155(18)	-33(9)	-17(9)	-35(7)
C(94A)	53(12)	41(10)	190(30)	2(13)	-32(14)	-27(9)
C(94B)	230(30)	260(40)	27(9)	-51(14)	46(14)	-220(30)

Table 32. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a-6C₉H₈O** (*trans*-Cinnamaldehyde).

	x	y	z	U(eq)
H(1A)	5012	1001	10181	24
H(6A)	9544	-1121	10923	82
H(6B)	9044	-684	11380	82
H(6C)	9150	-141	10796	82
H(7A)	7827	-411	9851	71
H(7B)	8813	-971	10013	71
H(7C)	8428	10	9872	71
H(8A)	7636	-1297	10820	65
H(8B)	8133	-1388	11392	65
H(8C)	8632	-1814	10931	65
H(9A)	8068	610	11227	40
H(12A)	6257	2969	11840	73
H(12B)	5795	2420	11803	73
H(12C)	5846	3042	11240	73
H(13A)	7619	2694	11451	87
H(13B)	7234	2741	10849	87
H(13C)	8066	1945	11179	87
H(14A)	7538	1700	12356	79
H(14B)	7988	949	12087	79
H(14C)	7108	1124	12318	79
H(15A)	5569	2122	10962	32
H(20A)	4079	1914	7590	69
H(20B)	4502	1428	8232	69
H(20C)	4864	1985	7829	69

H(21A)	3141	3979	7711	86
H(21B)	3248	3440	7281	86
H(21C)	4031	3528	7503	86
H(22A)	2549	3144	8381	73
H(22B)	3035	2158	8564	73
H(22C)	2634	2655	7920	73
H(23A)	4205	3837	8286	40
H(26A)	6040	3678	9604	84
H(26B)	5227	4056	9911	84
H(26C)	5560	4651	9520	84
H(27A)	4133	5511	8961	94
H(27B)	3792	4913	9337	94
H(27C)	3698	5102	8662	94
H(28A)	5897	3959	8524	85
H(28B)	5428	4925	8468	85
H(28C)	4995	4521	8162	85
H(29A)	5315	2840	9920	31
H(34A)	3493	-202	12312	66
H(34B)	4042	265	12354	66
H(34C)	4118	-156	11854	66
H(35A)	2186	1013	12323	70
H(35B)	1929	1900	11885	70
H(35C)	2690	1519	12378	70
H(36A)	2280	427	11512	66
H(36B)	2884	496	11044	66
H(36C)	2056	1298	11063	66
H(37A)	2738	2528	11652	35
H(40A)	3157	4412	10304	89
H(40B)	3982	4099	10728	89
H(40C)	3157	4903	10748	89
H(41A)	3256	3387	12032	75
H(41B)	3218	4280	11799	75
H(41C)	4043	3476	11778	75
H(42A)	1877	4303	10690	61
H(42B)	1910	4809	11115	61
H(42C)	1896	3940	11357	61
H(43A)	4164	2991	10456	31
H(10A)	6801	1585	9585	58
H(10B)	7347	2335	8578	55
H(10C)	7763	2124	9725	59
H(10D)	8182	2937	8315	91
H(10E)	9158	3469	8100	110
H(10F)	9898	3594	8819	86
H(10G)	9716	3130	9755	116
H(10H)	8790	2563	9985	102
H(20D)	2837	3083	9585	57
H(20E)	1041	3982	9608	55
H(20F)	2224	4553	9272	55
H(20G)	1848	6015	9071	53
H(20H)	859	7406	8889	59
H(20I)	-571	7761	8912	60
H(20J)	-1011	6720	9130	63
H(20K)	-29	5324	9312	59
H(30A)	5201	940	11786	49
H(30B)	6094	101	12928	50
H(30C)	4747	1664	12489	47
H(30D)	6330	471	13718	61
H(30E)	6294	770	14595	74
H(30F)	5108	1868	14767	70
H(30G)	3960	2673	14058	63
H(30H)	3998	2405	13169	55
H(1BA)	10184	5997	5105	22
H(6BA)	9487	7453	2707	64

H(6BB)	8830	7152	2549	64
H(6BC)	9439	6677	3134	64
H(7BA)	7549	9061	2863	82
H(7BB)	7723	8601	2378	82
H(7BC)	8385	8875	2568	82
H(8BA)	7352	7882	3523	74
H(8BB)	8053	6950	3629	74
H(8BC)	7512	7454	3021	74
H(9BA)	8414	9128	3436	35
H(12D)	8392	10289	4900	96
H(12E)	8778	9312	5171	96
H(12F)	7880	9810	4799	96
H(13D)	8177	10891	3843	64
H(13E)	7763	10339	3719	64
H(13F)	8572	10319	3433	64
H(14D)	9625	10192	4407	71
H(14E)	9973	9614	3996	71
H(14F)	10090	9211	4666	71
H(15B)	9676	8114	5023	28
H(20L)	13324	4256	4418	75
H(20M)	12675	3989	4748	75
H(20N)	13646	3352	4848	75
H(21D)	14354	4480	4917	79
H(21E)	14687	3589	5365	79
H(21F)	14388	4393	5582	79
H(22D)	12766	3772	5877	73
H(22E)	13508	3859	6164	73
H(22F)	13715	3123	5884	73
H(23B)	13502	5693	5047	35
H(26D)	12258	8514	4200	85
H(26E)	11502	8282	4306	85
H(26F)	12220	7820	3954	85
H(27D)	12627	8216	5268	77
H(27E)	12730	7366	5690	77
H(27F)	11832	8043	5361	77
H(28D)	13692	7545	4683	74
H(28E)	13685	6826	4453	74
H(28F)	13891	6671	5117	74
H(29B)	11096	7412	4927	29
H(34D)	7950	6085	6161	72
H(34E)	7507	6820	6445	72
H(34F)	7520	5946	6724	72
H(35D)	8981	6006	7698	91
H(35E)	8172	5857	7669	91
H(35F)	8107	6751	7380	91
H(36D)	9700	4790	7314	65
H(36E)	9360	4790	6714	65
H(36F)	8856	4710	7246	65
H(37B)	9202	6982	7116	39
H(40D)	9109	8901	6301	84
H(40E)	9390	9003	6881	84
H(40F)	8854	8510	6885	84
H(41D)	11322	7514	6564	66
H(41E)	10905	8381	6705	66
H(41F)	10617	8308	6115	66
H(42D)	10916	6876	7510	83
H(42E)	9972	7313	7639	83
H(42F)	10546	7772	7605	83
H(43B)	10610	7243	5852	29
H(40G)	10783	7224	3809	60
H(40H)	11499	7394	2748	63
H(40I)	10337	8584	3211	56
H(40J)	9724	10039	2682	84

H(40K)	9583	11123	1893	94
H(40L)	10404	10855	1147	76
H(40M)	11282	9491	1178	122
H(40N)	11440	8407	1975	115
H(50A)	11358	5393	7323	56
H(50B)	12321	5412	6375	53
H(50C)	12381	5870	7366	58
H(50D)	13119	6736	7339	97
H(50E)	14217	7049	7078	121
H(50F)	15093	6418	6448	117
H(50G)	14856	5484	6076	98
H(50H)	13729	5196	6330	75
H(60A)	8132	7853	5420	55
H(60B)	6333	8882	5244	53
H(60C)	7590	8907	5898	55
H(60D)	5333	9770	5678	77
H(60E)	4376	10923	5961	106
H(60F)	4872	11675	6358	118
H(60G)	6320	11268	6486	119
H(60H)	7272	10102	6237	86
H(91A)	14078	5647	2809	54
H(91B)	13434	5880	3261	54
H(92A)	13311	4948	2913	80
H(92B)	13146	5530	2279	80
H(92C)	12475	5801	2710	80
H(93A)	12922	7846	2534	216
H(93B)	13109	7221	3149	216
H(93C)	14056	6802	3002	76
H(93D)	14099	7035	2334	76
H(94A)	13975	7772	2695	150
H(94B)	14353	6885	2583	150
H(94C)	14250	6960	3216	150
H(94D)	13739	8023	2772	185
H(94E)	12863	7992	2809	185
H(94F)	13171	8209	2205	185

Table 33. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**·**6C**₁₀H₁₄O (Safranal). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	Site Occupancy
Na(1)	1051(1)	5823(1)	521(1)	29(1)	
Na(2)	-290(1)	5150(1)	-1288(1)	30(1)	
Na(3)	565(1)	3854(1)	204(1)	28(1)	
O(1)	1271(2)	4746(1)	784(1)	22(1)	
O(3)	13(2)	4072(1)	-921(1)	23(1)	
O(2)	429(2)	5944(1)	-652(1)	23(1)	
C(1)	1351(2)	4820(2)	-621(2)	17(1)	
C(2)	1920(2)	4443(2)	-87(2)	18(1)	
C(3)	1859(2)	4459(2)	610(2)	20(1)	
C(4)	2420(2)	4127(2)	1097(2)	22(1)	
C(5)	2394(2)	4117(2)	1865(2)	28(1)	
C(6)	1690(3)	3752(2)	1956(2)	35(1)	
C(7)	3062(3)	3747(3)	2307(2)	49(2)	
C(8)	2415(3)	4812(2)	2150(2)	38(1)	

C(9)	2981(2)	3802(2)	863(2)	25(1)
C(10)	3036(2)	3766(2)	178(2)	22(1)
C(11)	3678(2)	3419(2)	-66(2)	27(1)
C(12)	4119(3)	2964(3)	481(3)	47(1)
C(13)	4208(3)	3930(3)	-247(3)	48(1)
C(14)	3385(3)	3009(2)	-697(3)	44(1)
C(15)	2492(2)	4095(2)	-283(2)	22(1)
C(16)	1611(2)	5510(2)	-748(2)	19(1)
C(17)	1103(2)	6038(2)	-789(2)	20(1)
C(18)	1352(2)	6674(2)	-948(2)	23(1)
C(19)	850(2)	7277(2)	-973(2)	29(1)
C(20)	1208(3)	7899(2)	-1197(3)	46(1)
C(21)	108(2)	7180(2)	-1486(2)	35(1)
C(22)	711(3)	7411(2)	-254(2)	36(1)
C(23)	2073(2)	6739(2)	-1051(2)	24(1)
C(24)	2583(2)	6221(2)	-996(2)	24(1)
C(25)	3368(2)	6343(2)	-1123(2)	32(1)
C(26)	3846(3)	5748(3)	-1006(3)	61(2)
C(27)	3751(3)	6879(3)	-619(3)	53(2)
C(28)	3313(3)	6602(3)	-1848(3)	55(2)
C(29)	2335(2)	5617(2)	-837(2)	22(1)
C(30)	1101(2)	4432(2)	-1286(2)	18(1)
C(31)	444(2)	4043(2)	-1383(2)	20(1)
C(32)	260(2)	3654(2)	-1991(2)	23(1)
C(33)	-453(2)	3237(2)	-2143(2)	31(1)
C(34)	-525(3)	2834(3)	-2804(3)	49(2)
C(35)	-473(3)	2750(2)	-1563(3)	45(1)
C(36)	-1133(3)	3692(3)	-2251(3)	42(1)
C(37)	734(2)	3673(2)	-2458(2)	26(1)
C(38)	1363(2)	4067(2)	-2378(2)	24(1)
C(39)	1883(2)	4075(2)	-2892(2)	28(1)
C(40)	1580(3)	3664(3)	-3529(3)	53(2)
C(41)	2648(3)	3791(3)	-2539(3)	53(2)
C(42)	1987(3)	4774(2)	-3122(3)	51(2)
C(43)	1524(2)	4445(2)	-1794(2)	22(1)
O(101)	2190(2)	6250(2)	916(2)	47(1)
C(101)	2803(3)	6022(2)	895(2)	39(1)
C(102)	3513(3)	6320(2)	1211(2)	32(1)
C(103)	3534(3)	7009(2)	1519(3)	40(1)
C(104)	4308(3)	7309(3)	1552(3)	51(2)
C(105)	4931(3)	6856(3)	1824(3)	52(2)
C(106)	4843(3)	6221(3)	1706(3)	46(1)
C(107)	4135(3)	5952(2)	1319(2)	40(1)
C(108)	3370(3)	6946(3)	2237(3)	59(2)
C(109)	2960(3)	7475(3)	1096(4)	70(2)
C(110)	4190(3)	5255(3)	1084(3)	61(2)
O(201)	-307(2)	5307(2)	-2411(2)	44(1)
C(201)	120(3)	5674(3)	-2617(3)	42(1)
C(202)	82(3)	5866(2)	-3332(2)	34(1)
C(203)	-535(3)	5578(2)	-3900(2)	36(1)
C(204)	-651(3)	6024(3)	-4534(3)	46(1)
C(205)	46(3)	6278(3)	-4695(3)	52(2)
C(206)	642(3)	6371(2)	-4197(3)	46(1)
C(207)	640(3)	6227(2)	-3493(3)	38(1)
C(208)	-282(3)	4904(2)	-4063(3)	50(1)
C(209)	-1293(3)	5527(3)	-3699(3)	50(1)
C(210)	1303(3)	6500(3)	-2977(3)	52(2)
O(301)	1144(2)	2868(2)	287(2)	41(1)
C(301)	1419(3)	2662(2)	-172(3)	39(1)
C(302)	1776(3)	2023(2)	-188(2)	33(1)
C(303)	1978(3)	1616(2)	466(2)	36(1)
C(304)	2599(3)	1138(3)	405(3)	56(2)
C(305)	2487(4)	809(3)	-277(3)	64(2)

C(306)	2139(3)	1112(3)	-827(3)	55(2)	
C(307)	1848(3)	1770(3)	-801(3)	40(1)	
C(308)	1274(3)	1247(3)	558(3)	58(2)	
C(309)	2270(3)	2028(3)	1107(3)	52(2)	
C(310)	1638(3)	2109(3)	-1489(3)	59(2)	
O(401)	554(6)	-408(4)	1099(5)	71(3)	0.5
C(401)	-32(9)	-521(7)	1396(7)	82(5)	0.5
C(402)	-323(10)	-72(10)	1785(9)	132(7)	0.5
C(403)	828(6)	-883(5)	723(6)	48(3)	0.5
C(404)	1446(7)	-751(5)	471(6)	53(3)	0.5

Table 34. Bond lengths [Å] and angles [deg] for **3a**·6C₁₀H₁₄O (Safranal).

Na(1)-O(101)	2.250(4)	C(19)-C(21)	1.534(6)
Na(1)-O(3)#1	2.270(3)	C(19)-C(22)	1.534(6)
Na(1)-O(1)	2.282(3)	C(19)-C(20)	1.542(6)
Na(1)-O(2)	2.391(3)	C(23)-C(24)	1.403(6)
Na(1)-C(17)	2.673(4)	C(24)-C(29)	1.377(6)
Na(1)-C(16)	2.994(4)	C(24)-C(25)	1.533(6)
Na(1)-Na(2)#1	3.026(2)	C(25)-C(26)	1.491(7)
Na(1)-Na(3)#1	3.084(2)	C(25)-C(28)	1.524(7)
Na(1)-Na(3)	4.147(2)	C(25)-C(27)	1.553(7)
Na(1)-Na(2)	4.151(2)	C(30)-C(43)	1.400(6)
Na(2)-O(1)#1	2.249(3)	C(30)-C(31)	1.424(5)
Na(2)-O(201)	2.256(4)	C(31)-C(32)	1.430(6)
Na(2)-O(2)	2.300(3)	C(32)-C(37)	1.402(6)
Na(2)-O(3)	2.356(3)	C(32)-C(33)	1.539(6)
Na(2)-C(31)	2.663(4)	C(33)-C(35)	1.534(7)
Na(2)-C(30)	2.945(4)	C(33)-C(36)	1.536(7)
Na(2)-Na(1)#1	3.026(2)	C(33)-C(34)	1.537(6)
Na(2)-Na(3)#1	3.089(2)	C(37)-C(38)	1.391(6)
Na(2)-C(201)	3.097(6)	C(38)-C(43)	1.377(6)
Na(2)-C(1)	3.100(4)	C(38)-C(39)	1.543(6)
Na(2)-C(17)	3.124(4)	C(39)-C(40)	1.527(7)
Na(2)-Na(3)	4.049(2)	C(39)-C(42)	1.527(6)
Na(3)-O(2)#1	2.231(3)	C(39)-C(41)	1.545(7)
Na(3)-O(301)	2.271(4)	O(101)-C(101)	1.227(6)
Na(3)-O(3)	2.303(3)	C(101)-C(102)	1.457(7)
Na(3)-O(1)	2.392(3)	C(102)-C(107)	1.346(7)
Na(3)-C(3)	2.649(4)	C(102)-C(103)	1.536(6)
Na(3)-C(2)	2.929(4)	C(103)-C(108)	1.529(7)
Na(3)-C(301)	3.077(6)	C(103)-C(109)	1.534(7)
Na(3)-Na(1)#1	3.084(2)	C(103)-C(104)	1.537(7)
Na(3)-Na(2)#1	3.089(2)	C(104)-C(105)	1.482(8)
Na(3)-C(1)	3.114(4)	C(105)-C(106)	1.324(7)
O(1)-C(3)	1.336(5)	C(106)-C(107)	1.472(7)
O(1)-Na(2)#1	2.249(3)	C(107)-C(110)	1.511(7)
O(3)-C(31)	1.335(5)	O(201)-C(201)	1.219(6)
O(3)-Na(1)#1	2.270(3)	C(201)-C(202)	1.467(7)
O(2)-C(17)	1.336(5)	C(202)-C(207)	1.355(7)
O(2)-Na(3)#1	2.231(3)	C(202)-C(203)	1.541(6)
C(1)-C(16)	1.528(5)	C(203)-C(208)	1.513(7)
C(1)-C(30)	1.533(5)	C(203)-C(209)	1.531(7)
C(1)-C(2)	1.534(5)	C(203)-C(204)	1.538(7)
C(2)-C(15)	1.392(6)	C(204)-C(205)	1.478(8)
C(2)-C(3)	1.418(6)	C(205)-C(206)	1.326(7)
C(3)-C(4)	1.430(5)	C(206)-C(207)	1.437(7)
C(4)-C(9)	1.388(6)	C(207)-C(210)	1.523(7)
C(4)-C(5)	1.542(6)	O(301)-C(301)	1.210(6)
C(5)-C(8)	1.531(6)	C(301)-C(302)	1.468(7)

C(5)-C(6)	1.536(6)	C(302)-C(307)	1.358(7)
C(5)-C(7)	1.548(6)	C(302)-C(303)	1.526(6)
C(9)-C(10)	1.393(6)	C(303)-C(304)	1.527(7)
C(10)-C(15)	1.380(5)	C(303)-C(309)	1.531(7)
C(10)-C(11)	1.541(6)	C(303)-C(308)	1.541(7)
C(11)-C(14)	1.515(6)	C(304)-C(305)	1.494(8)
C(11)-C(13)	1.521(6)	C(305)-C(306)	1.303(8)
C(11)-C(12)	1.531(6)	C(306)-C(307)	1.454(7)
C(16)-C(29)	1.395(6)	C(307)-C(310)	1.515(7)
C(16)-C(17)	1.419(6)	O(401)-C(401)	1.353(17)
C(17)-C(18)	1.437(6)	O(401)-C(403)	1.384(13)
C(18)-C(23)	1.387(6)	C(401)-C(402)	1.38(2)
C(18)-C(19)	1.536(6)	C(403)-C(404)	1.363(15)
O(101)-Na(1)-O(3)#1	130.09(14)	Na(2)#1-O(1)-Na(3)	83.41(11)
O(101)-Na(1)-O(1)	100.84(13)	Na(1)-O(1)-Na(3)	125.04(12)
O(3)#1-Na(1)-O(1)	97.77(12)	C(31)-O(3)-Na(1)#1	157.6(3)
O(101)-Na(1)-O(2)	121.28(13)	C(31)-O(3)-Na(3)	117.5(2)
O(3)#1-Na(1)-O(2)	93.78(11)	Na(1)#1-O(3)-Na(3)	84.79(11)
O(1)-Na(1)-O(2)	110.55(11)	C(31)-O(3)-Na(2)	87.8(2)
O(101)-Na(1)-C(17)	93.25(13)	Na(1)#1-O(3)-Na(2)	81.68(11)
O(3)#1-Na(1)-C(17)	122.61(13)	Na(3)-O(3)-Na(2)	120.71(13)
O(1)-Na(1)-C(17)	110.10(13)	C(17)-O(2)-Na(3)#1	157.7(3)
O(2)-Na(1)-C(17)	29.93(10)	C(17)-O(2)-Na(2)	115.9(2)
O(101)-Na(1)-C(16)	85.44(13)	Na(3)#1-O(2)-Na(2)	85.96(11)
O(3)#1-Na(1)-C(16)	142.32(12)	C(17)-O(2)-Na(1)	86.8(2)
O(1)-Na(1)-C(16)	84.97(11)	Na(3)#1-O(2)-Na(1)	83.63(11)
O(2)-Na(1)-C(16)	51.17(10)	Na(2)-O(2)-Na(1)	124.50(13)
C(17)-Na(1)-C(16)	28.28(11)	C(16)-C(1)-C(30)	112.5(3)
O(101)-Na(1)-Na(2)#1	124.88(11)	C(16)-C(1)-C(2)	113.0(3)
O(3)#1-Na(1)-Na(2)#1	50.39(8)	C(30)-C(1)-C(2)	112.1(3)
O(1)-Na(1)-Na(2)#1	47.64(8)	C(16)-C(1)-Na(2)	92.1(2)
O(2)-Na(1)-Na(2)#1	112.83(9)	C(30)-C(1)-Na(2)	69.8(2)
C(17)-Na(1)-Na(2)#1	135.97(11)	C(2)-C(1)-Na(2)	150.0(3)
C(16)-Na(1)-Na(2)#1	124.33(10)	C(16)-C(1)-Na(3)	150.4(3)
O(101)-Na(1)-Na(3)#1	144.22(12)	C(30)-C(1)-Na(3)	92.4(2)
O(3)#1-Na(1)-Na(3)#1	48.06(8)	C(2)-C(1)-Na(3)	68.7(2)
O(1)-Na(1)-Na(3)#1	114.93(9)	Na(2)-C(1)-Na(3)	81.34(10)
O(2)-Na(1)-Na(3)#1	45.98(8)	C(15)-C(2)-C(3)	120.6(4)
C(17)-Na(1)-Na(3)#1	74.61(10)	C(15)-C(2)-C(1)	120.4(3)
C(16)-Na(1)-Na(3)#1	96.69(9)	C(3)-C(2)-C(1)	119.1(3)
Na(2)#1-Na(1)-Na(3)#1	83.02(6)	C(15)-C(2)-Na(3)	124.6(3)
O(101)-Na(1)-Na(3)	125.81(12)	C(3)-C(2)-Na(3)	64.5(2)
O(3)#1-Na(1)-Na(3)	88.46(9)	C(1)-C(2)-Na(3)	82.1(2)
O(1)-Na(1)-Na(3)	28.18(7)	O(1)-C(3)-C(2)	120.0(3)
O(2)-Na(1)-Na(3)	84.79(8)	O(1)-C(3)-C(4)	122.5(4)
C(17)-Na(1)-Na(3)	93.58(10)	C(2)-C(3)-C(4)	117.4(4)
C(16)-Na(1)-Na(3)	76.38(9)	O(1)-C(3)-Na(3)	64.19(19)
Na(2)#1-Na(1)-Na(3)	47.96(5)	C(2)-C(3)-Na(3)	86.6(2)
Na(3)#1-Na(1)-Na(3)	89.00(5)	C(4)-C(3)-Na(3)	117.1(3)
O(101)-Na(1)-Na(2)	140.39(11)	C(9)-C(4)-C(3)	118.6(4)
O(3)#1-Na(1)-Na(2)	86.64(8)	C(9)-C(4)-C(5)	120.5(4)
O(1)-Na(1)-Na(2)	85.63(8)	C(3)-C(4)-C(5)	120.9(4)
O(2)-Na(1)-Na(2)	27.16(7)	C(8)-C(5)-C(6)	111.3(4)
C(17)-Na(1)-Na(2)	48.79(9)	C(8)-C(5)-C(4)	110.7(4)
C(16)-Na(1)-Na(2)	55.97(8)	C(6)-C(5)-C(4)	109.1(3)
Na(2)#1-Na(1)-Na(2)	88.26(5)	C(8)-C(5)-C(7)	106.8(4)
Na(3)#1-Na(1)-Na(2)	47.80(4)	C(6)-C(5)-C(7)	106.2(4)
Na(3)-Na(1)-Na(2)	58.42(4)	C(4)-C(5)-C(7)	112.7(4)
O(1)#1-Na(2)-O(201)	125.84(13)	C(4)-C(9)-C(10)	124.5(4)
O(1)#1-Na(2)-O(2)	96.12(11)	C(15)-C(10)-C(9)	115.9(4)
O(201)-Na(2)-O(2)	109.48(13)	C(15)-C(10)-C(11)	120.5(4)
O(1)#1-Na(2)-O(3)	96.24(11)	C(9)-C(10)-C(11)	123.5(4)

O(201)-Na(2)-O(3)	113.25(13)	C(14)-C(11)-C(13)	108.5(4)
O(2)-Na(2)-O(3)	114.86(11)	C(14)-C(11)-C(12)	107.3(4)
O(1)#1-Na(2)-C(31)	125.19(13)	C(13)-C(11)-C(12)	108.6(4)
O(201)-Na(2)-C(31)	87.26(13)	C(14)-C(11)-C(10)	110.9(3)
O(2)-Na(2)-C(31)	113.63(13)	C(13)-C(11)-C(10)	109.1(4)
O(3)-Na(2)-C(31)	30.05(11)	C(12)-C(11)-C(10)	112.3(4)
O(1)#1-Na(2)-C(30)	145.26(12)	C(10)-C(15)-C(2)	122.9(4)
O(201)-Na(2)-C(30)	84.42(12)	C(29)-C(16)-C(17)	120.3(4)
O(2)-Na(2)-C(30)	87.47(11)	C(29)-C(16)-C(1)	120.3(4)
O(3)-Na(2)-C(30)	51.95(10)	C(17)-C(16)-C(1)	119.3(3)
C(31)-Na(2)-C(30)	28.87(11)	C(29)-C(16)-Na(1)	125.5(3)
O(1)#1-Na(2)-Na(1)#1	48.56(8)	C(17)-C(16)-Na(1)	63.2(2)
O(201)-Na(2)-Na(1)#1	133.20(12)	C(1)-C(16)-Na(1)	83.3(2)
O(2)-Na(2)-Na(1)#1	117.26(10)	O(2)-C(17)-C(16)	120.2(4)
O(3)-Na(2)-Na(1)#1	47.93(8)	O(2)-C(17)-C(18)	121.9(4)
C(31)-Na(2)-Na(1)#1	76.68(10)	C(16)-C(17)-C(18)	117.9(4)
C(30)-Na(2)-Na(1)#1	99.38(9)	O(2)-C(17)-Na(1)	63.3(2)
O(1)#1-Na(2)-Na(3)#1	50.27(8)	C(16)-C(17)-Na(1)	88.6(2)
O(201)-Na(2)-Na(3)#1	129.11(11)	C(18)-C(17)-Na(1)	116.3(3)
O(2)-Na(2)-Na(3)#1	46.09(8)	O(2)-C(17)-Na(2)	41.47(17)
O(3)-Na(2)-Na(3)#1	117.61(9)	C(16)-C(17)-Na(2)	93.3(2)
C(31)-Na(2)-Na(3)#1	140.40(11)	C(18)-C(17)-Na(2)	137.3(3)
C(30)-Na(2)-Na(3)#1	126.70(10)	Na(1)-C(17)-Na(2)	91.14(12)
Na(1)#1-Na(2)-Na(3)#1	85.38(6)	C(23)-C(18)-C(17)	118.5(4)
O(1)#1-Na(2)-C(201)	135.41(13)	C(23)-C(18)-C(19)	120.2(4)
O(201)-Na(2)-C(201)	19.23(13)	C(17)-C(18)-C(19)	121.2(4)
O(2)-Na(2)-C(201)	90.73(13)	C(21)-C(19)-C(22)	110.4(4)
O(3)-Na(2)-C(201)	120.43(13)	C(21)-C(19)-C(18)	111.1(4)
C(31)-Na(2)-C(201)	90.93(13)	C(22)-C(19)-C(18)	109.3(4)
C(30)-Na(2)-C(201)	78.85(12)	C(21)-C(19)-C(20)	106.6(4)
Na(1)#1-Na(2)-C(201)	151.94(12)	C(22)-C(19)-C(20)	106.8(4)
Na(3)#1-Na(2)-C(201)	118.41(11)	C(18)-C(19)-C(20)	112.5(4)
O(1)#1-Na(2)-C(1)	128.68(12)	C(18)-C(23)-C(24)	123.9(4)
O(201)-Na(2)-C(1)	105.45(13)	C(29)-C(24)-C(23)	116.6(4)
O(2)-Na(2)-C(1)	61.61(10)	C(29)-C(24)-C(25)	123.6(4)
O(3)-Na(2)-C(1)	61.15(10)	C(23)-C(24)-C(25)	119.8(4)
C(31)-Na(2)-C(1)	52.05(11)	C(26)-C(25)-C(28)	110.6(4)
C(30)-Na(2)-C(1)	29.23(10)	C(26)-C(25)-C(24)	112.5(4)
Na(1)#1-Na(2)-C(1)	98.57(9)	C(28)-C(25)-C(24)	109.7(4)
Na(3)#1-Na(2)-C(1)	97.46(9)	C(26)-C(25)-C(27)	107.8(4)
C(201)-Na(2)-C(1)	93.08(13)	C(28)-C(25)-C(27)	107.4(4)
O(1)#1-Na(2)-C(17)	118.73(12)	C(24)-C(25)-C(27)	108.8(4)
O(201)-Na(2)-C(17)	94.16(13)	C(24)-C(29)-C(16)	122.8(4)
O(2)-Na(2)-C(17)	22.62(10)	C(43)-C(30)-C(31)	119.7(4)
O(3)-Na(2)-C(17)	108.82(11)	C(43)-C(30)-C(1)	120.5(3)
C(31)-Na(2)-C(17)	97.24(12)	C(31)-C(30)-C(1)	119.8(3)
C(30)-Na(2)-C(17)	68.86(11)	C(43)-C(30)-Na(2)	127.0(3)
Na(1)#1-Na(2)-C(17)	130.95(10)	C(31)-C(30)-Na(2)	64.5(2)
Na(3)#1-Na(2)-C(17)	68.66(9)	C(1)-C(30)-Na(2)	81.0(2)
C(201)-Na(2)-C(17)	74.97(13)	O(3)-C(31)-C(30)	119.3(3)
C(1)-Na(2)-C(17)	48.27(10)	O(3)-C(31)-C(32)	122.8(4)
O(1)#1-Na(2)-Na(3)	87.46(8)	C(30)-C(31)-C(32)	117.8(4)
O(201)-Na(2)-Na(3)	138.18(11)	O(3)-C(31)-Na(2)	62.12(19)
O(2)-Na(2)-Na(3)	88.23(8)	C(30)-C(31)-Na(2)	86.6(2)
O(3)-Na(2)-Na(3)	29.28(7)	C(32)-C(31)-Na(2)	120.1(3)
C(31)-Na(2)-Na(3)	51.03(9)	C(37)-C(32)-C(31)	118.8(4)
C(30)-Na(2)-Na(3)	58.04(8)	C(37)-C(32)-C(33)	120.2(4)
Na(1)#1-Na(2)-Na(3)	49.10(4)	C(31)-C(32)-C(33)	121.0(4)
Na(3)#1-Na(2)-Na(3)	90.72(5)	C(35)-C(33)-C(36)	110.6(4)
C(201)-Na(2)-Na(3)	136.89(11)	C(35)-C(33)-C(34)	106.8(4)
C(1)-Na(2)-Na(3)	49.49(8)	C(36)-C(33)-C(34)	106.5(4)
C(17)-Na(2)-Na(3)	89.02(8)	C(35)-C(33)-C(32)	111.5(4)
O(2)#1-Na(3)-O(301)	123.04(13)	C(36)-C(33)-C(32)	108.8(4)

O(2)#1-Na(3)-O(3)	97.26(11)	C(34)-C(33)-C(32)	112.6(4)
O(301)-Na(3)-O(3)	110.18(13)	C(38)-C(37)-C(32)	123.8(4)
O(2)#1-Na(3)-O(1)	94.04(11)	C(43)-C(38)-C(37)	116.6(4)
O(301)-Na(3)-O(1)	116.46(12)	C(43)-C(38)-C(39)	120.4(4)
O(3)-Na(3)-O(1)	113.95(11)	C(37)-C(38)-C(39)	123.0(4)
O(2)#1-Na(3)-C(3)	123.13(13)	C(40)-C(39)-C(42)	108.3(4)
O(301)-Na(3)-C(3)	91.00(13)	C(40)-C(39)-C(38)	112.3(4)
O(3)-Na(3)-C(3)	112.87(13)	C(42)-C(39)-C(38)	110.0(4)
O(1)-Na(3)-C(3)	30.20(11)	C(40)-C(39)-C(41)	108.1(4)
O(2)#1-Na(3)-C(2)	143.39(12)	C(42)-C(39)-C(41)	109.3(4)
O(301)-Na(3)-C(2)	88.60(12)	C(38)-C(39)-C(41)	108.8(4)
O(3)-Na(3)-C(2)	86.79(11)	C(38)-C(43)-C(30)	123.3(4)
O(1)-Na(3)-C(2)	52.11(10)	C(101)-O(101)-Na(1)	129.1(3)
C(3)-Na(3)-C(2)	28.90(11)	O(101)-C(101)-C(102)	124.7(5)
O(2)#1-Na(3)-C(301)	138.22(13)	C(107)-C(102)-C(101)	119.0(4)
O(301)-Na(3)-C(301)	19.66(12)	C(107)-C(102)-C(103)	120.2(4)
O(3)-Na(3)-C(301)	93.25(13)	C(101)-C(102)-C(103)	120.1(4)
O(1)-Na(3)-C(301)	118.12(12)	C(108)-C(103)-C(109)	108.6(5)
C(3)-Na(3)-C(301)	88.59(13)	C(108)-C(103)-C(102)	107.7(4)
C(2)-Na(3)-C(301)	77.30(12)	C(109)-C(103)-C(102)	113.3(4)
O(2)#1-Na(3)-Na(1)#1	50.39(8)	C(108)-C(103)-C(104)	110.8(4)
O(301)-Na(3)-Na(1)#1	127.87(11)	C(109)-C(103)-C(104)	107.2(4)
O(3)-Na(3)-Na(1)#1	47.15(8)	C(102)-C(103)-C(104)	109.2(4)
O(1)-Na(3)-Na(1)#1	115.62(9)	C(105)-C(104)-C(103)	113.6(5)
C(3)-Na(3)-Na(1)#1	138.94(11)	C(106)-C(105)-C(104)	119.6(5)
C(2)-Na(3)-Na(1)#1	126.22(10)	C(105)-C(106)-C(107)	121.5(5)
C(301)-Na(3)-Na(1)#1	122.98(11)	C(102)-C(107)-C(106)	119.9(5)
O(2)#1-Na(3)-Na(2)#1	47.95(8)	C(102)-C(107)-C(110)	126.1(5)
O(301)-Na(3)-Na(2)#1	132.75(11)	C(106)-C(107)-C(110)	114.0(5)
O(3)-Na(3)-Na(2)#1	116.87(10)	C(201)-O(201)-Na(2)	123.2(3)
O(1)-Na(3)-Na(2)#1	46.32(8)	O(201)-C(201)-C(202)	126.3(5)
C(3)-Na(3)-Na(2)#1	75.25(10)	C(202)-C(201)-Na(2)	162.7(4)
C(2)-Na(3)-Na(2)#1	97.92(9)	C(207)-C(202)-C(201)	119.5(4)
C(301)-Na(3)-Na(2)#1	149.39(11)	C(207)-C(202)-C(203)	120.7(4)
Na(1)#1-Na(3)-Na(2)#1	84.51(6)	C(201)-C(202)-C(203)	119.3(4)
O(2)#1-Na(3)-C(1)	127.06(12)	C(208)-C(203)-C(209)	109.4(4)
O(301)-Na(3)-C(1)	109.90(13)	C(208)-C(203)-C(204)	111.1(4)
O(3)-Na(3)-C(1)	61.28(10)	C(209)-C(203)-C(204)	106.3(4)
O(1)-Na(3)-C(1)	60.45(10)	C(208)-C(203)-C(202)	107.2(4)
C(3)-Na(3)-C(1)	51.64(11)	C(209)-C(203)-C(202)	113.7(4)
C(2)-Na(3)-C(1)	29.20(10)	C(204)-C(203)-C(202)	109.3(4)
C(301)-Na(3)-C(1)	93.31(13)	C(205)-C(204)-C(203)	114.3(5)
Na(1)#1-Na(3)-C(1)	97.02(9)	C(206)-C(205)-C(204)	120.2(5)
Na(2)#1-Na(3)-C(1)	96.48(9)	C(205)-C(206)-C(207)	122.1(5)
O(2)#1-Na(3)-Na(2)	87.17(9)	C(202)-C(207)-C(206)	120.1(5)
O(301)-Na(3)-Na(2)	137.58(11)	C(202)-C(207)-C(210)	125.1(5)
O(3)-Na(3)-Na(2)	30.01(8)	C(206)-C(207)-C(210)	114.8(5)
O(1)-Na(3)-Na(2)	86.68(8)	C(301)-O(301)-Na(3)	121.2(3)
C(3)-Na(3)-Na(2)	95.83(10)	O(301)-C(301)-C(302)	125.9(5)
C(2)-Na(3)-Na(2)	78.36(9)	C(302)-C(301)-Na(3)	164.9(4)
C(301)-Na(3)-Na(2)	118.56(11)	C(307)-C(302)-C(301)	119.2(5)
Na(1)#1-Na(3)-Na(2)	47.88(5)	C(307)-C(302)-C(303)	120.6(4)
Na(2)#1-Na(3)-Na(2)	89.28(5)	C(301)-C(302)-C(303)	119.8(4)
C(1)-Na(3)-Na(2)	49.17(8)	C(302)-C(303)-C(304)	109.4(4)
O(2)#1-Na(3)-Na(1)	85.81(9)	C(302)-C(303)-C(309)	113.2(4)
O(301)-Na(3)-Na(1)	140.37(10)	C(304)-C(303)-C(309)	106.5(4)
O(3)-Na(3)-Na(1)	89.82(9)	C(302)-C(303)-C(308)	108.1(4)
O(1)-Na(3)-Na(1)	26.78(7)	C(304)-C(303)-C(308)	110.7(4)
C(3)-Na(3)-Na(1)	49.37(9)	C(309)-C(303)-C(308)	108.9(4)
C(2)-Na(3)-Na(1)	57.74(8)	C(305)-C(304)-C(303)	113.6(5)
C(301)-Na(3)-Na(1)	134.69(10)	C(306)-C(305)-C(304)	120.1(5)
Na(1)#1-Na(3)-Na(1)	91.00(5)	C(305)-C(306)-C(307)	121.9(5)
Na(2)#1-Na(3)-Na(1)	46.67(4)	C(302)-C(307)-C(306)	119.4(5)

C(1)-Na(3)-Na(1)	49.82(8)	C(302)-C(307)-C(310)	125.9(5)
Na(2)-Na(3)-Na(1)	60.85(4)	C(306)-C(307)-C(310)	114.7(5)
C(3)-O(1)-Na(2)#1	157.4(3)	C(401)-O(401)-C(403)	122.1(10)
C(3)-O(1)-Na(1)	118.5(2)	O(401)-C(401)-C(402)	124.8(14)
Na(2)#1-O(1)-Na(1)	83.80(11)	C(404)-C(403)-O(401)	119.1(9)
C(3)-O(1)-Na(3)	85.6(2)		

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

Table 35. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**·6C₁₀H₁₄O (Safranal). The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Na(1)	25(1)	31(1)	30(1)	0(1)	5(1)	-2(1)
Na(2)	30(1)	30(1)	31(1)	2(1)	8(1)	3(1)
Na(3)	25(1)	30(1)	31(1)	-2(1)	7(1)	0(1)
O(1)	20(2)	28(2)	20(2)	1(1)	5(1)	7(1)
O(3)	23(2)	28(2)	20(2)	-5(1)	8(1)	-5(1)
O(2)	18(2)	21(2)	30(2)	3(1)	8(1)	0(1)
C(1)	15(2)	17(2)	20(2)	-2(2)	4(2)	0(2)
C(2)	16(2)	17(2)	20(2)	0(2)	1(2)	-4(2)
C(3)	17(2)	18(2)	23(2)	0(2)	1(2)	0(2)
C(4)	21(2)	26(2)	19(2)	2(2)	2(2)	1(2)
C(5)	31(3)	31(3)	22(2)	1(2)	4(2)	10(2)
C(6)	49(3)	35(3)	26(3)	8(2)	17(2)	12(2)
C(7)	43(3)	74(4)	26(3)	8(3)	-1(2)	26(3)
C(8)	42(3)	45(3)	26(3)	-3(2)	3(2)	1(2)
C(9)	21(2)	28(2)	23(2)	2(2)	-3(2)	2(2)
C(10)	18(2)	20(2)	27(2)	2(2)	4(2)	-1(2)
C(11)	22(2)	26(2)	32(3)	0(2)	5(2)	4(2)
C(12)	35(3)	57(3)	49(3)	17(3)	12(2)	26(3)
C(13)	36(3)	44(3)	72(4)	-6(3)	30(3)	-2(2)
C(14)	36(3)	45(3)	49(3)	-17(3)	5(2)	15(2)
C(15)	24(2)	21(2)	22(2)	-1(2)	6(2)	-1(2)
C(16)	20(2)	21(2)	16(2)	-2(2)	1(2)	-3(2)
C(17)	19(2)	22(2)	19(2)	-2(2)	0(2)	-1(2)
C(18)	23(2)	23(2)	22(2)	2(2)	2(2)	-3(2)
C(19)	28(3)	19(2)	40(3)	5(2)	7(2)	3(2)
C(20)	39(3)	24(3)	73(4)	15(3)	12(3)	1(2)
C(21)	29(3)	34(3)	41(3)	9(2)	2(2)	5(2)
C(22)	37(3)	25(3)	46(3)	-7(2)	8(2)	-2(2)
C(23)	21(2)	21(2)	29(2)	3(2)	4(2)	-7(2)
C(24)	23(2)	28(2)	22(2)	3(2)	5(2)	-1(2)
C(25)	17(2)	42(3)	35(3)	9(2)	5(2)	-3(2)
C(26)	26(3)	54(4)	109(5)	27(4)	29(3)	2(3)
C(27)	31(3)	62(4)	65(4)	1(3)	7(3)	-14(3)
C(28)	42(3)	73(4)	56(4)	13(3)	25(3)	-9(3)
C(29)	18(2)	21(2)	25(2)	2(2)	3(2)	2(2)
C(30)	19(2)	15(2)	20(2)	2(2)	3(2)	3(2)
C(31)	20(2)	18(2)	21(2)	1(2)	5(2)	4(2)
C(32)	25(2)	22(2)	22(2)	1(2)	3(2)	0(2)
C(33)	31(3)	34(3)	27(3)	-11(2)	7(2)	-11(2)
C(34)	51(3)	55(4)	44(3)	-19(3)	14(3)	-23(3)
C(35)	55(3)	38(3)	43(3)	-10(3)	11(3)	-21(3)

C(36)	24(3)	58(3)	41(3)	-8(3)	1(2)	-6(2)
C(37)	30(3)	24(2)	21(2)	-5(2)	1(2)	2(2)
C(38)	26(2)	26(2)	19(2)	1(2)	5(2)	5(2)
C(39)	33(3)	29(3)	25(2)	-5(2)	13(2)	4(2)
C(40)	61(4)	69(4)	37(3)	-10(3)	28(3)	-4(3)
C(41)	42(3)	75(4)	48(3)	-2(3)	22(3)	14(3)
C(42)	65(4)	48(3)	48(3)	8(3)	34(3)	-5(3)
C(43)	21(2)	24(2)	21(2)	1(2)	3(2)	-1(2)
O(101)	39(2)	56(2)	43(2)	-7(2)	5(2)	-12(2)
C(101)	48(3)	38(3)	31(3)	-5(2)	6(2)	-12(3)
C(102)	38(3)	32(3)	27(3)	-3(2)	9(2)	-11(2)
C(103)	41(3)	33(3)	47(3)	-14(2)	11(2)	-12(2)
C(104)	50(4)	47(3)	55(4)	-15(3)	11(3)	-22(3)
C(105)	43(3)	75(4)	39(3)	-19(3)	10(3)	-23(3)
C(106)	37(3)	59(4)	42(3)	-4(3)	10(2)	-9(3)
C(107)	48(3)	40(3)	34(3)	-7(2)	17(2)	-10(3)
C(108)	59(4)	70(4)	54(4)	-35(3)	24(3)	-19(3)
C(109)	63(4)	40(3)	98(5)	-3(3)	-1(4)	-4(3)
C(110)	67(4)	41(3)	80(4)	-17(3)	27(4)	-5(3)
O(201)	47(2)	46(2)	41(2)	9(2)	13(2)	3(2)
C(201)	43(3)	39(3)	38(3)	-5(3)	-1(3)	10(3)
C(202)	35(3)	31(3)	36(3)	-7(2)	7(2)	4(2)
C(203)	40(3)	38(3)	30(3)	-5(2)	8(2)	1(2)
C(204)	58(4)	43(3)	38(3)	-3(3)	8(3)	-3(3)
C(205)	75(4)	44(3)	39(3)	-2(3)	14(3)	-4(3)
C(206)	52(3)	34(3)	56(4)	-3(3)	21(3)	-10(3)
C(207)	41(3)	33(3)	41(3)	-5(2)	9(2)	6(2)
C(208)	57(4)	40(3)	53(4)	-11(3)	11(3)	-2(3)
C(209)	42(3)	55(4)	48(3)	-8(3)	1(3)	-2(3)
C(210)	46(3)	50(3)	58(4)	-9(3)	4(3)	-12(3)
O(301)	39(2)	39(2)	46(2)	-6(2)	14(2)	2(2)
C(301)	35(3)	38(3)	42(3)	2(2)	5(2)	-7(2)
C(302)	32(3)	30(3)	39(3)	2(2)	9(2)	2(2)
C(303)	39(3)	32(3)	38(3)	0(2)	8(2)	3(2)
C(304)	59(4)	48(4)	60(4)	2(3)	9(3)	14(3)
C(305)	75(4)	45(4)	78(5)	-7(3)	26(4)	25(3)
C(306)	60(4)	51(4)	57(4)	-17(3)	18(3)	6(3)
C(307)	35(3)	48(3)	37(3)	-5(3)	6(2)	-5(2)
C(308)	62(4)	49(4)	65(4)	13(3)	20(3)	-2(3)
C(309)	59(4)	52(3)	42(3)	1(3)	4(3)	1(3)
C(310)	56(4)	82(5)	38(3)	-10(3)	8(3)	9(3)
O(401)	95(8)	45(5)	66(6)	-17(4)	1(5)	-20(5)
C(401)	91(11)	69(10)	60(9)	-34(8)	-41(8)	0(9)
C(402)	139(17)	168(19)	80(12)	-64(13)	2(11)	-20(15)
C(403)	47(7)	26(6)	53(7)	-21(5)	-27(6)	-11(5)
C(404)	70(8)	32(6)	58(8)	-15(5)	14(6)	-15(6)

Table 36. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**·**6C**₁₀**H**₁₄**O** (Safranal).

	x	y	z	U(eq)
H(1A)	907	4872	-425	21
H(6A)	1256	3979	1713	53
H(6B)	1679	3733	2435	53
H(6C)	1695	3317	1778	53
H(7A)	3012	3742	2776	74
H(7B)	3518	3963	2275	74
H(7C)	3071	3307	2143	74
H(8A)	2004	5058	1893	57
H(8B)	2875	5019	2114	57
H(8C)	2379	4797	2623	57
H(9A)	3347	3593	1186	30
H(12A)	4498	2745	301	70
H(12B)	3788	2647	610	70
H(12C)	4347	3216	876	70
H(13A)	4615	3716	-389	71
H(13B)	4396	4196	147	71
H(13C)	3946	4199	-614	71
H(14A)	3796	2815	-854	66
H(14B)	3105	3280	-1052	66
H(14C)	3068	2670	-585	66
H(15A)	2510	4084	-745	27
H(20A)	867	8258	-1222	68
H(20B)	1323	7830	-1640	68
H(20C)	1658	7997	-870	68
H(21A)	-138	6798	-1363	53
H(21B)	201	7127	-1939	53
H(21C)	-204	7555	-1478	53
H(22A)	470	7040	-102	55
H(22B)	399	7789	-267	55
H(22C)	1179	7488	58	55
H(23A)	2228	7150	-1162	29
H(26A)	3624	5410	-1317	91
H(26B)	3888	5600	-543	91
H(26C)	4332	5850	-1083	91
H(27A)	4224	6988	-721	80
H(27B)	3824	6719	-157	80
H(27C)	3441	7261	-666	80
H(28A)	3114	6269	-2173	82
H(28B)	3800	6725	-1908	82
H(28C)	2991	6977	-1919	82
H(29A)	2664	5266	-786	26
H(34A)	-965	2568	-2867	74
H(34B)	-95	2560	-2771	74
H(34C)	-561	3124	-3189	74
H(35A)	-944	2527	-1652	68
H(35B)	-412	2981	-1136	68
H(35C)	-77	2439	-1537	68
H(36A)	-1581	3436	-2344	63
H(36B)	-1125	3978	-2632	63
H(36C)	-1117	3948	-1845	63
H(37A)	620	3406	-2843	31
H(40A)	1089	3813	-3740	79
H(40B)	1557	3214	-3399	79
H(40C)	1903	3706	-3848	79
H(41A)	2990	3828	-2842	80