H(41B)	2592	3340	-2430	80
H(41C)	2839	4030	-2125	80
H(42A)	1515	4945	-3358	76
H(42B)	2330	4777	-3424	76
H(42C)	2179	5040	-2728	76
H(43A)	1933	4723	-1735	27
H(10A)	2815	5631	660	47
H(10B)	4346	7446	1095	61
H(10C)	4359	7695	1840	61
H(10D)	5380	7016	2076	63
H(10E)	5237	5939	1872	55
H(10F)	2887	6753	2205	89
H(10G)	3379	7371	2442	89
H(10H)	3742	6674	2514	89
H(10I)	2471	7364	1158	104
H(10J)	2977	7438	620	104
H(10K)	3075	7916	1247	104
H(11A)	3718	5121	813	91
H(11B)	4322	4975	1477	91
H(11C)	4564	5226	815	91
H(20D)	508	5849	-2290	50
H(20E)	-920	5782	-4928	56
H(20F)	-960	6391	-4462	56
H(20G)	68	6373	-5146	63
H(20H)	1074	6535	-4308	55
H(20I)	-655	4709	-4416	75
H(20J)	-208	4637	-3658	75
H(20K)	178	4938	-4218	75
H(20L)	-1667	5407	-4094	75
H(20M)	-1419	5941	-3529	75
H(20N)	-1270	5201	-3350	75
H(21D)	1249	6397	-2520	79
H(21E)	1322	6965	-3029	79
H(21F)	1755	6309	-3057	79
H(30A)	1402	2934	-549	47
H(30B)	3070	1371	488	67
H(30C)	2632	807	759	67
H(30D)	2666	388	-310	77
H(30E)	2075	901	-1248	66
H(30F)	1101	973	167	87
H(30G)	893	1556	600	87
H(30H)	1391	983	964	87
H(30I)	2647	2321	1021	78
H(30J)	2478	1745	1483	78
H(30K)	1867	2274	1219	78
H(31A)	1520	2558	-1421	88
H(31B)	1212	1897	-1765	88
H(31C)	2049	2088	-1717	88
H(40D)	98	-902	1685	98
H(40M)	-442	-651	1029	98
H(40E)	-576	-298	2091	199
H(40F)	-669	207	1488	199
H(40G)	74	186	2046	199
H(40H)	933	-1268	1010	57
H(40I)	430	-998	339	57
H(40J)	1664	-1153	361	80
H(40K)	1801	-518	809	80
H(40L)	1310	-489	65	80

Table 37. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3a·6$C_8H_{14}O$** (cyclohexyl methyl ketone). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Na(1)	2511(1)	6929(1)	1406(1)	27(1)
O(1)	3569(1)	7680(1)	1329(1)	24(1)
C(1)	3333	6667	845(1)	22(1)
C(2)	3607(1)	7373(1)	733(1)	23(1)
C(3)	3681(1)	7839(1)	990(1)	22(1)
C(4)	3885(1)	8479(1)	870(1)	26(1)
C(5)	3960(1)	9006(1)	1127(1)	32(1)
C(6)	4157(2)	9645(1)	941(1)	52(1)
C(7)	4482(1)	9138(1)	1398(1)	41(1)
C(8)	3320(1)	8804(1)	1312(1)	39(1)
C(9)	4007(1)	8616(1)	514(1)	30(1)
C(10)	3956(1)	8172(1)	262(1)	30(1)
C(11)	4040(1)	8339(1)	-134(1)	36(1)
C(12)	4566(1)	9028(1)	-203(1)	59(1)
C(13)	4190(2)	7889(2)	-342(1)	60(1)
C(14)	3407(1)	8265(1)	-270(1)	48(1)
C(15)	3763(1)	7559(1)	383(1)	27(1)
O(101)	1908(1)	7172(1)	1063(1)	54(1)
C(101)	1761(1)	7279(1)	776(1)	42(1)
C(102)	1082(1)	7131(1)	708(1)	51(1)
C(103)	790(1)	6641(2)	415(1)	67(1)
C(104)	103(2)	6464(2)	330(1)	73(1)
C(105)	-296(2)	6281(2)	670(1)	80(1)
C(106)	-18(2)	6762(2)	948(1)	76(1)
C(107)	668(1)	6934(2)	1024(1)	58(1)
C(108)	2237(1)	7573(1)	486(1)	48(1)
Na(1B)	-1125(1)	9285(1)	-263(1)	29(1)
O(1B)	-387(1)	8959(1)	-340(1)	27(1)
C(1B)	0	10000	-829(1)	26(1)
C(2B)	-172(1)	9316(1)	-940(1)	27(1)
C(3B)	-378(1)	8825(1)	-680(1)	25(1)
C(4B)	-569(1)	8188(1)	-798(1)	30(1)
C(5B)	-809(1)	7628(1)	-538(1)	34(1)
C(6B)	-999(1)	6988(1)	-720(1)	49(1)
C(7B)	-286(1)	7747(1)	-269(1)	40(1)
C(8B)	-1410(1)	7548(1)	-349(1)	39(1)
C(9B)	-551(1)	8078(1)	-1158(1)	36(1)
C(10B)	-338(1)	8556(1)	-1412(1)	39(1)
C(11B)	-361(1)	8397(1)	-1806(1)	49(1)
C(12B)	-81(3)	7966(3)	-1873(1)	114(2)
C(13B)	-1044(2)	8077(2)	-1928(1)	85(1)
C(14B)	30(2)	9004(2)	-2030(1)	87(1)
C(15B)	-143(1)	9169(1)	-1293(1)	35(1)
O(201)	-2071(1)	8740(1)	-565(1)	53(1)
C(201)	-2323(1)	8575(1)	-852(1)	45(1)
C(202)	-3006(1)	8439(1)	-910(1)	47(1)
C(203)	-3353(1)	8394(1)	-570(1)	52(1)
C(204)	-4028(2)	8272(2)	-637(1)	69(1)
C(205)	-4014(2)	8784(2)	-869(1)	79(1)
C(206)	-3677(2)	8828(2)	-1212(1)	75(1)
C(207)	-2998(2)	8948(2)	-1152(1)	62(1)
C(208)	-1970(1)	8511(2)	-1159(1)	62(1)

Table 38. Bond lengths [A] and angles [deg] for **3a·6$C_8H_{14}O$** (cyclohexyl methyl ketone).

Na(1)-O(101)	2.2393(18)	C(4)-C(9)	1.389(3)
Na(1)-O(1)#1	2.2754(14)	C(4)-C(5)	1.539(3)
Na(1)-O(1)	2.2911(15)	C(5)-C(7)	1.531(3)
Na(1)-O(1)#2	2.3315(15)	C(5)-C(8)	1.536(3)
Na(1)-C(3)#2	2.8046(19)	C(5)-C(6)	1.537(3)
Na(1)-C(3)	3.0132(19)	C(9)-C(10)	1.397(3)
Na(1)-Na(1)#1	3.0833(11)	C(10)-C(15)	1.388(3)
Na(1)-Na(1)#3	3.0833(11)	C(10)-C(11)	1.542(3)
Na(1)-Na(1)#4	4.0946(13)	C(11)-C(12)	1.527(3)
Na(1)-Na(1)#2	4.0946(13)	C(11)-C(13)	1.527(3)
O(1)-C(3)	1.333(2)	C(11)-C(14)	1.533(3)
O(1)-Na(1)#3	2.2754(14)	O(101)-C(101)	1.211(3)
O(1)-Na(1)#4	2.3315(15)	C(101)-C(108)	1.489(4)
C(1)-C(2)	1.546(2)	C(101)-C(102)	1.513(3)
C(1)-C(2)#2	1.546(2)	C(102)-C(107)	1.481(4)
C(1)-C(2)#4	1.546(2)	C(102)-C(103)	1.517(4)
C(2)-C(15)	1.394(3)	C(103)-C(104)	1.525(4)
C(2)-C(3)	1.430(3)	C(104)-C(105)	1.535(5)
C(3)-C(4)	1.440(3)	C(105)-C(106)	1.461(5)
C(3)-Na(1)#4	2.8046(19)	C(106)-C(107)	1.518(4)
Na(1B)-O(201)	2.2896(18)	C(4B)-C(9B)	1.396(3)
Na(1B)-O(1B)	2.2946(15)	C(4B)-C(5B)	1.534(3)
Na(1B)-O(1B)#5	2.2985(15)	C(5B)-C(7B)	1.533(3)
Na(1B)-O(1B)#6	2.3282(15)	C(5B)-C(8B)	1.539(3)
Na(1B)-C(3B)#6	2.830(2)	C(5B)-C(6B)	1.539(3)
Na(1B)-C(3B)	2.996(2)	C(9B)-C(10B)	1.390(3)
Na(1B)-Na(1B)#5	3.1064(11)	C(10B)-C(15B)	1.382(3)
Na(1B)-Na(1B)#7	3.1064(11)	C(10B)-C(11B)	1.542(3)
Na(1B)-Na(1B)#6	4.1184(13)	C(11B)-C(13B)	1.501(4)
Na(1B)-Na(1B)#8	4.1184(13)	C(11B)-C(12B)	1.513(4)
O(1B)-C(3B)	1.335(2)	C(11B)-C(14B)	1.541(4)
O(1B)-Na(1B)#7	2.2985(15)	O(201)-C(201)	1.216(3)
O(1B)-Na(1B)#8	2.3282(15)	C(201)-C(208)	1.496(4)
C(1B)-C(2B)	1.543(2)	C(201)-C(202)	1.525(3)
C(1B)-C(2B)#8	1.543(2)	C(202)-C(203)	1.514(4)
C(1B)-C(2B)#6	1.543(2)	C(202)-C(207)	1.525(4)
C(2B)-C(15B)	1.398(3)	C(203)-C(204)	1.524(4)
C(2B)-C(3B)	1.426(3)	C(204)-C(205)	1.505(5)
C(3B)-C(4B)	1.436(3)	C(205)-C(206)	1.511(5)
C(3B)-Na(1B)#8	2.830(2)	C(206)-C(207)	1.532(4)

O(101)-Na(1)-O(1)#1	129.42(7)	C(2)-C(1)-C(2)#2	112.86(11)
O(101)-Na(1)-O(1)	109.38(7)	C(2)-C(1)-C(2)#4	112.86(11)
O(1)#1-Na(1)-O(1)	95.71(5)	C(2)#2-C(1)-C(2)#4	112.86(11)
O(101)-Na(1)-O(1)#2	113.85(7)	C(15)-C(2)-C(3)	119.40(17)
O(1)#1-Na(1)-O(1)#2	94.60(5)	C(15)-C(2)-C(1)	120.81(18)
O(1)-Na(1)-O(1)#2	112.15(6)	C(3)-C(2)-C(1)	119.76(17)
O(101)-Na(1)-C(3)#2	89.15(7)	O(1)-C(3)-C(2)	120.37(16)
O(1)#1-Na(1)-C(3)#2	122.10(6)	O(1)-C(3)-C(4)	121.73(16)
O(1)-Na(1)-C(3)#2	111.27(6)	C(2)-C(3)-C(4)	117.90(16)
O(1)#2-Na(1)-C(3)#2	28.21(5)	O(1)-C(3)-Na(1)#4	55.76(8)
O(101)-Na(1)-C(3)	89.93(7)	C(2)-C(3)-Na(1)#4	89.83(11)
O(1)#1-Na(1)-C(3)	120.23(5)	C(4)-C(3)-Na(1)#4	124.97(12)
O(1)-Na(1)-C(3)	24.62(5)	O(1)-C(3)-Na(1)	45.73(8)
O(1)#2-Na(1)-C(3)	109.10(5)	C(2)-C(3)-Na(1)	94.68(11)
C(3)#2-Na(1)-C(3)	96.89(8)	C(4)-C(3)-Na(1)	129.77(12)
O(101)-Na(1)-Na(1)#1	135.33(6)	Na(1)#4-C(3)-Na(1)	89.39(6)

O(1)#1-Na(1)-Na(1)#1	47.75(4)	C(9)-C(4)-C(3)	118.80(17)
O(1)-Na(1)-Na(1)#1	115.28(4)	C(9)-C(4)-C(5)	119.82(17)
O(1)#2-Na(1)-Na(1)#1	47.22(3)	C(3)-C(4)-C(5)	121.38(16)
C(3)#2-Na(1)-Na(1)#1	74.35(4)	C(7)-C(5)-C(8)	110.52(18)
C(3)-Na(1)-Na(1)#1	132.42(4)	C(7)-C(5)-C(6)	106.88(19)
O(101)-Na(1)-Na(1)#3	131.24(6)	C(8)-C(5)-C(6)	106.66(19)
O(1)#1-Na(1)-Na(1)#3	48.77(4)	C(7)-C(5)-C(4)	110.06(17)
O(1)-Na(1)-Na(1)#3	47.31(3)	C(8)-C(5)-C(4)	110.01(17)
O(1)#2-Na(1)-Na(1)#3	114.81(4)	C(6)-C(5)-C(4)	112.63(17)
C(3)#2-Na(1)-Na(1)#3	136.45(4)	C(4)-C(9)-C(10)	123.96(18)
C(3)-Na(1)-Na(1)#3	71.56(4)	C(15)-C(10)-C(9)	116.29(17)
Na(1)#1-Na(1)-Na(1)#3	83.21(3)	C(15)-C(10)-C(11)	122.25(18)
O(101)-Na(1)-Na(1)#4	133.12(6)	C(9)-C(10)-C(11)	121.14(18)
O(1)#1-Na(1)-Na(1)#4	87.02(4)	C(12)-C(11)-C(13)	108.7(2)
O(1)-Na(1)-Na(1)#4	27.91(4)	C(12)-C(11)-C(14)	107.9(2)
O(1)#2-Na(1)-Na(1)#4	86.53(4)	C(13)-C(11)-C(14)	108.5(2)
C(3)#2-Na(1)-Na(1)#4	94.11(4)	C(12)-C(11)-C(10)	112.47(19)
C(3)-Na(1)-Na(1)#4	43.23(4)	C(13)-C(11)-C(10)	111.42(18)
Na(1)#1-Na(1)-Na(1)#4	90.0	C(14)-C(11)-C(10)	107.82(17)
Na(1)#3-Na(1)-Na(1)#4	48.396(17)	C(10)-C(15)-C(2)	123.54(18)
O(101)-Na(1)-Na(1)#2	136.28(6)	C(101)-O(101)-Na(1)	151.10(18)
O(1)#1-Na(1)-Na(1)#2	86.45(4)	O(101)-C(101)-C(108)	121.9(2)
O(1)-Na(1)-Na(1)#2	87.04(4)	O(101)-C(101)-C(102)	119.9(2)
O(1)#2-Na(1)-Na(1)#2	27.39(4)	C(108)-C(101)-C(102)	118.1(2)
C(3)#2-Na(1)-Na(1)#2	47.38(4)	C(107)-C(102)-C(101)	114.5(2)
C(3)-Na(1)-Na(1)#2	91.00(4)	C(107)-C(102)-C(103)	111.7(2)
Na(1)#1-Na(1)-Na(1)#2	48.396(17)	C(101)-C(102)-C(103)	109.6(2)
Na(1)#3-Na(1)-Na(1)#2	90.0	C(102)-C(103)-C(104)	112.9(3)
Na(1)#4-Na(1)-Na(1)#2	60.0	C(103)-C(104)-C(105)	109.9(3)
C(3)-O(1)-Na(1)#3	161.53(12)	C(106)-C(105)-C(104)	113.9(3)
C(3)-O(1)-Na(1)	109.64(11)	C(105)-C(106)-C(107)	111.0(3)
Na(1)#3-O(1)-Na(1)	84.94(5)	C(102)-C(107)-C(106)	113.6(3)
C(3)-O(1)-Na(1)#4	96.03(10)	O(201)-Na(1B)-O(1B)	117.44(7)
Na(1)#3-O(1)-Na(1)#4	84.02(5)	O(201)-Na(1B)-O(1B)#5	124.47(7)
Na(1)-O(1)-Na(1)#4	124.70(6)		
O(1B)-Na(1B)-O(1B)#5	95.20(6)	C(2B)-C(1B)-C(2B)#8	112.89(11)
O(201)-Na(1B)-O(1B)#6	111.65(6)	C(2B)-C(1B)-C(2B)#6	112.89(11)
O(1B)-Na(1B)-O(1B)#6	110.83(7)	C(2B)#8-C(1B)-C(2B)#6	112.89(11)
O(1B)#5-Na(1B)-O(1B)#6	94.28(6)	C(15B)-C(2B)-C(3B)	119.44(18)
O(201)-Na(1B)-C(3B)#6	89.33(6)	C(15B)-C(2B)-C(1B)	120.8(2)
O(1B)-Na(1B)-C(3B)#6	110.15(6)	C(3B)-C(2B)-C(1B)	119.72(18)
O(1B)#5-Na(1B)-C(3B)#6	121.58(6)	O(1B)-C(3B)-C(2B)	120.54(17)
O(1B)#6-Na(1B)-C(3B)#6	27.89(5)	O(1B)-C(3B)-C(4B)	121.70(17)
O(201)-Na(1B)-C(3B)	97.69(6)	C(2B)-C(3B)-C(4B)	117.77(17)
O(1B)-Na(1B)-C(3B)	25.02(5)	O(1B)-C(3B)-Na(1B)#8	54.67(9)
O(1B)#5-Na(1B)-C(3B)	120.08(6)	C(2B)-C(3B)-Na(1B)#8	91.17(11)
O(1B)#6-Na(1B)-C(3B)	108.42(6)	C(4B)-C(3B)-Na(1B)#8	124.59(13)
C(3B)#6-Na(1B)-C(3B)	96.28(8)	O(1B)-C(3B)-Na(1B)	46.63(8)
O(201)-Na(1B)-Na(1B)#5	127.81(6)	C(2B)-C(3B)-Na(1B)	94.70(12)
O(1B)-Na(1B)-Na(1B)#5	114.73(4)	C(4B)-C(3B)-Na(1B)	129.05(13)
O(1B)#5-Na(1B)-Na(1B)#5	47.39(4)	Na(1B)#8-C(3B)-Na(1B)	89.92(6)
O(1B)#6-Na(1B)-Na(1B)#5	47.42(3)	C(9B)-C(4B)-C(3B)	118.92(19)
C(3B)#6-Na(1B)-Na(1B)#5	74.20(4)	C(9B)-C(4B)-C(5B)	119.85(18)
C(3B)-Na(1B)-Na(1B)#5	132.54(4)	C(3B)-C(4B)-C(5B)	121.20(17)
O(201)-Na(1B)-Na(1B)#7	133.78(6)	C(7B)-C(5B)-C(4B)	110.61(17)
O(1B)-Na(1B)-Na(1B)#7	47.50(3)	C(7B)-C(5B)-C(8B)	110.38(18)
O(1B)#5-Na(1B)-Na(1B)#7	48.23(4)	C(4B)-C(5B)-C(8B)	109.17(17)
O(1B)#6-Na(1B)-Na(1B)#7	114.35(4)	C(7B)-C(5B)-C(6B)	106.87(19)
C(3B)#6-Na(1B)-Na(1B)#7	135.71(4)	C(4B)-C(5B)-C(6B)	112.63(18)
C(3B)-Na(1B)-Na(1B)#7	71.99(4)	C(8B)-C(5B)-C(6B)	107.11(18)
Na(1B)#5-Na(1B)-Na(1B)#7	83.04(3)	C(10B)-C(9B)-C(4B)	123.74(19)
O(201)-Na(1B)-Na(1B)#6	135.92(6)	C(15B)-C(10B)-C(9B)	116.52(19)

O(1B)-Na(1B)-Na(1B)#6	86.33(4)	C(15B)-C(10B)-C(11B)	122.4(2)
O(1B)#5-Na(1B)-Na(1B)#6	85.86(4)	C(9B)-C(10B)-C(11B)	121.0(2)
O(1B)#6-Na(1B)-Na(1B)#6	26.80(4)	C(13B)-C(11B)-C(12B)	110.3(3)
C(3B)#6-Na(1B)-Na(1B)#6	46.68(4)	C(13B)-C(11B)-C(14B)	108.1(3)
C(3B)-Na(1B)-Na(1B)#6	90.95(4)	C(12B)-C(11B)-C(14B)	106.8(3)
Na(1B)#5-Na(1B)-Na(1B)#6	48.479(17)	C(13B)-C(11B)-C(10B)	108.6(2)
Na(1B)#7-Na(1B)-Na(1B)#6	90.0	C(12B)-C(11B)-C(10B)	111.2(2)
O(201)-Na(1B)-Na(1B)#8	141.06(6)	C(14B)-C(11B)-C(10B)	111.7(2)
O(1B)-Na(1B)-Na(1B)#8	27.23(4)	C(10B)-C(15B)-C(2B)	123.5(2)
O(1B)#5-Na(1B)-Na(1B)#8	86.34(4)	C(201)-O(201)-Na(1B)	146.02(19)
O(1B)#6-Na(1B)-Na(1B)#8	85.92(4)	O(201)-C(201)-C(208)	121.0(2)
C(3B)#6-Na(1B)-Na(1B)#8	93.39(4)	O(201)-C(201)-C(202)	120.7(2)
C(3B)-Na(1B)-Na(1B)#8	43.40(4)	C(208)-C(201)-C(202)	118.4(2)
Na(1B)#5-Na(1B)-Na(1B)#8	90.0	C(203)-C(202)-C(207)	110.9(2)
Na(1B)#7-Na(1B)-Na(1B)#8	48.479(17)	C(203)-C(202)-C(201)	112.9(2)
Na(1B)#6-Na(1B)-Na(1B)#8	60.0	C(207)-C(202)-C(201)	109.7(2)
C(3B)-O(1B)-Na(1B)	108.36(11)	C(202)-C(203)-C(204)	111.7(2)
C(3B)-O(1B)-Na(1B)#7	161.11(12)	C(205)-C(204)-C(203)	110.9(3)
Na(1B)-O(1B)-Na(1B)#7	85.11(5)	C(204)-C(205)-C(206)	110.7(3)
C(3B)-O(1B)-Na(1B)#8	97.44(11)	C(205)-C(206)-C(207)	111.8(3)
Na(1B)-O(1B)-Na(1B)#8	125.97(7)	C(202)-C(207)-C(206)	110.9(3)
Na(1B)#7-O(1B)-Na(1B)#8	84.35(5)		

Symmetry transformations used to generate equivalent atoms:
#1 x-y+2/3,x+1/3,-z+1/3 #2 -y+1,x-y+1,z
#3 y-1/3,-x+y+1/3,-z+1/3 #4 -x+y,-x+1,z
#5 y-1,-x+y,-z #6 -x+y-1,-x+1,z #7 x-y+1,x+1,-z
#8 -y+1,x-y+2,z

Table 39. Anisotropic displacement parameters (A^2 x 10^3)
for **3a·6$C_8H_{14}O$** (cyclohexyl methyl ketone).
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Na(1)	28(1)	29(1)	24(1)	1(1)	-1(1)	15(1)
O(1)	29(1)	24(1)	20(1)	2(1)	0(1)	13(1)
C(1)	24(1)	24(1)	17(1)	0	0	12(1)
C(2)	21(1)	26(1)	22(1)	2(1)	-1(1)	11(1)
C(3)	21(1)	25(1)	21(1)	2(1)	-1(1)	11(1)
C(4)	26(1)	25(1)	28(1)	3(1)	1(1)	13(1)
C(5)	39(1)	23(1)	33(1)	3(1)	2(1)	15(1)
C(6)	81(2)	28(1)	46(1)	5(1)	7(1)	27(1)
C(7)	39(1)	32(1)	44(1)	-7(1)	-5(1)	12(1)
C(8)	45(1)	39(1)	41(1)	-4(1)	1(1)	27(1)
C(9)	31(1)	27(1)	33(1)	8(1)	2(1)	14(1)
C(10)	29(1)	34(1)	25(1)	7(1)	3(1)	16(1)
C(11)	42(1)	41(1)	25(1)	10(1)	5(1)	22(1)
C(12)	57(2)	57(2)	37(1)	21(1)	7(1)	9(1)
C(13)	97(2)	82(2)	27(1)	18(1)	21(1)	65(2)
C(14)	54(2)	63(2)	31(1)	10(1)	-3(1)	31(1)
C(15)	28(1)	30(1)	23(1)	1(1)	1(1)	15(1)
O(101)	60(1)	69(1)	49(1)	-2(1)	-16(1)	44(1)
C(101)	42(1)	43(1)	49(1)	0(1)	-10(1)	26(1)
C(102)	43(1)	57(2)	53(2)	6(1)	-5(1)	26(1)
C(103)	50(2)	73(2)	73(2)	-22(2)	-4(1)	26(2)
C(104)	52(2)	61(2)	92(2)	-7(2)	-26(2)	18(2)
C(105)	42(2)	69(2)	117(3)	-12(2)	7(2)	19(2)

C(106)	49(2)	80(2)	91(3)	4(2)	10(2)	27(2)
C(107)	50(2)	60(2)	66(2)	4(1)	2(1)	31(1)
C(108)	40(1)	49(1)	60(2)	-2(1)	-3(1)	25(1)
Na(1B)	30(1)	31(1)	27(1)	-1(1)	-3(1)	15(1)
O(1B)	30(1)	28(1)	22(1)	-2(1)	0(1)	14(1)
C(1B)	30(1)	30(1)	17(2)	0	0	15(1)
C(2B)	27(1)	31(1)	23(1)	-4(1)	-2(1)	14(1)
C(3B)	23(1)	30(1)	24(1)	-5(1)	-2(1)	13(1)
C(4B)	26(1)	29(1)	33(1)	-6(1)	-3(1)	13(1)
C(5B)	32(1)	27(1)	40(1)	-4(1)	1(1)	13(1)
C(6B)	54(2)	30(1)	57(2)	-7(1)	8(1)	16(1)
C(7B)	40(1)	36(1)	47(1)	4(1)	0(1)	21(1)
C(8B)	32(1)	33(1)	45(1)	-2(1)	4(1)	10(1)
C(9B)	36(1)	35(1)	37(1)	-16(1)	-7(1)	17(1)
C(10B)	44(1)	46(1)	27(1)	-12(1)	-5(1)	24(1)
C(11B)	66(2)	57(2)	28(1)	-16(1)	-7(1)	33(1)
C(12B)	216(5)	171(4)	39(2)	-34(2)	-15(2)	159(5)
C(13B)	82(2)	114(3)	36(2)	-21(2)	-20(2)	31(2)
C(14B)	121(3)	80(2)	30(1)	-15(1)	12(2)	29(2)
C(15B)	42(1)	41(1)	23(1)	-2(1)	-1(1)	22(1)
O(201)	45(1)	53(1)	53(1)	-5(1)	-19(1)	19(1)
C(201)	40(1)	38(1)	48(1)	0(1)	-12(1)	13(1)
C(202)	43(1)	45(1)	48(1)	-4(1)	-14(1)	18(1)
C(203)	47(2)	54(2)	51(2)	5(1)	-6(1)	22(1)
C(204)	53(2)	73(2)	77(2)	6(2)	0(2)	29(2)
C(205)	67(2)	90(3)	94(3)	12(2)	-2(2)	49(2)
C(206)	73(2)	88(2)	75(2)	16(2)	-19(2)	48(2)
C(207)	63(2)	68(2)	56(2)	13(1)	-6(1)	32(2)
C(208)	47(2)	73(2)	58(2)	1(2)	-5(1)	24(2)

Table 40. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3a·6C$_6$H$_{14}$O** (cyclohexyl methyl ketone).

	x	y	z	U(eq)
H(1A)	3333	6667	1102	26
H(6A)	4205	9959	1112	78
H(6B)	3833	9585	774	78
H(6C)	4557	9789	821	78
H(7A)	4505	9445	1567	61
H(7B)	4887	9305	1281	61
H(7C)	4382	8747	1516	61
H(8A)	3373	9131	1475	59
H(8B)	3184	8410	1437	59
H(8C)	3004	8743	1139	59
H(9A)	4129	9029	439	36
H(12A)	4588	9116	-451	89
H(12B)	4969	9085	-125	89
H(12C)	4472	9317	-78	89
H(13A)	4270	8024	-584	90
H(13B)	3832	7461	-330	90
H(13C)	4562	7899	-245	90
H(14A)	3449	8374	-516	72
H(14B)	3305	8544	-141	72
H(14C)	3071	7829	-239	72
H(15A)	3737	7256	222	32
H(10A)	1110	7527	621	61

H(10B)	798	6257	483	81
H(10C)	1050	6811	205	81
H(10D)	-82	6107	167	88
H(10E)	99	6825	219	88
H(10F)	-720	6209	614	96
H(10G)	-345	5881	757	96
H(10H)	-272	6599	1160	91
H(10I)	-27	7144	876	91
H(10J)	849	7280	1195	69
H(10K)	666	6567	1130	69
H(10L)	2646	7879	583	72
H(10M)	2098	7786	325	72
H(10N)	2275	7246	364	72
H(1BA)	0	10000	-571	31
H(6BA)	-634	7021	-842	74
H(6BB)	-1337	6888	-885	74
H(6BC)	-1143	6654	-547	74
H(7BA)	-143	8151	-155	60
H(7BB)	68	7751	-388	60
H(7BC)	-456	7411	-96	60
H(8BA)	-1298	7921	-209	59
H(8BB)	-1581	7178	-199	59
H(8BC)	-1725	7494	-521	59
H(9BA)	-690	7661	-1231	44
H(12D)	-54	7916	-2122	171
H(12E)	-352	7555	-1767	171
H(12F)	339	8155	-1771	171
H(13D)	-1065	7975	-2173	128
H(13E)	-1210	8361	-1892	128
H(13F)	-1294	7691	-1795	128
H(14D)	27	8885	-2271	130
H(14E)	464	9231	-1946	130
H(14F)	-156	9274	-2012	130
H(15B)	16	9500	-1456	42
H(20A)	-3243	8025	-1030	56
H(20B)	-3112	8790	-439	62
H(20C)	-3376	8049	-427	62
H(20D)	-4281	7858	-748	82
H(20E)	-4229	8264	-414	82
H(20F)	-3794	9193	-749	95
H(20G)	-4449	8687	-917	95
H(20H)	-3657	9174	-1353	90
H(20I)	-3923	8433	-1343	90
H(20J)	-2809	8941	-1376	75
H(20K)	-2736	9368	-1048	75
H(20L)	-1661	8401	-1076	93
H(20M)	-1755	8909	-1284	93
H(20N)	-2267	8180	-1313	93

Table 41. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3a·4C$_{11}$H$_{14}$O·Et$_2$O** (pivalophenone).
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Na(1)	253(1)	4104(1)	3305(1)	26(1)
Na(2)	-757(1)	3661(1)	5422(1)	26(1)
Na(3)	-1340(1)	5755(1)	4654(1)	26(1)
O(1)	-687(1)	5211(1)	3455(1)	23(1)
O(2)	-75(1)	3244(1)	4259(1)	23(1)
O(3)	-1634(1)	4884(1)	5372(1)	24(1)
C(1)	-1882(1)	3705(1)	3488(1)	20(1)
C(2)	-2310(2)	4208(1)	2884(1)	20(1)
C(3)	-1652(2)	4918(1)	2875(1)	21(1)
C(4)	-2084(2)	5327(1)	2257(1)	24(1)
C(5)	-1430(2)	6121(2)	2230(2)	29(1)
C(6)	-515(2)	5829(2)	2004(2)	33(1)
C(7)	-2010(2)	6420(2)	1485(2)	44(1)
C(8)	-1073(2)	6980(2)	3176(2)	33(1)
C(9)	-3106(2)	5002(2)	1699(2)	28(1)
C(10)	-3755(2)	4312(2)	1712(1)	27(1)
C(11)	-4878(2)	3972(2)	1064(2)	34(1)
C(12)	-5450(2)	3264(2)	1254(3)	65(1)
C(13)	-4974(2)	3509(2)	44(2)	60(1)
C(14)	-5380(2)	4787(2)	1208(2)	52(1)
C(15)	-3335(2)	3939(1)	2324(1)	25(1)
C(16)	-1595(1)	2830(1)	2940(1)	21(1)
C(17)	-682(2)	2637(1)	3393(1)	21(1)
C(18)	-436(2)	1803(1)	2879(1)	23(1)
C(19)	546(2)	1558(1)	3319(2)	28(1)
C(20)	651(2)	622(2)	2668(2)	43(1)
C(21)	1455(2)	2299(2)	3531(2)	34(1)
C(22)	588(2)	1497(2)	4228(2)	35(1)
C(23)	-1104(2)	1222(2)	1971(2)	29(1)
C(24)	-2006(2)	1402(2)	1517(1)	28(1)
C(25)	-2707(2)	711(2)	513(2)	36(1)
C(26)	-3035(2)	-240(2)	474(2)	55(1)
C(27)	-3660(2)	1037(2)	165(2)	55(1)
C(28)	-2145(2)	615(2)	-152(2)	48(1)
C(29)	-2219(2)	2221(1)	2022(1)	24(1)
C(30)	-2590(1)	3518(1)	3957(1)	20(1)
C(31)	-2454(2)	4176(1)	4871(1)	22(1)
C(32)	-3204(2)	4031(1)	5234(2)	27(1)
C(33)	-3130(2)	4736(2)	6199(2)	38(1)
C(34)	-4031(3)	4479(2)	6439(2)	66(1)
C(35)	-2172(2)	4775(2)	6968(2)	49(1)
C(36)	-3127(2)	5698(2)	6210(2)	51(1)
C(37)	-3996(2)	3246(2)	4697(2)	30(1)
C(38)	-4115(2)	2574(1)	3822(2)	26(1)
C(39)	-5007(2)	1717(2)	3285(2)	32(1)
C(40)	-5998(2)	2024(2)	3103(2)	60(1)
C(41)	-4993(2)	1063(2)	2347(2)	44(1)
C(42)	-4967(2)	1166(2)	3867(2)	53(1)
C(43)	-3395(2)	2733(1)	3472(1)	23(1)
O(101)	365(1)	3242(1)	1794(1)	44(1)
C(101)	222(2)	3038(2)	971(2)	38(1)
C(102)	-602(2)	3339(2)	423(2)	39(1)

C(103)	-1501(2)	3276(2)	571(2)	51(1)
C(104)	-2304(2)	3519(2)	71(3)	67(1)
C(105)	-2213(3)	3854(2)	-552(3)	71(1)
C(106)	-1315(3)	3949(2)	-682(2)	63(1)
C(107)	-519(2)	3682(2)	-207(2)	48(1)
C(108)	853(2)	2450(2)	504(2)	46(1)
C(109)	229(2)	1783(2)	-519(2)	59(1)
C(110)	1736(2)	3111(3)	557(2)	74(1)
C(111)	1267(4)	1907(3)	1042(3)	92(1)
O(201)	-1538(1)	2510(1)	5747(1)	46(1)
C(201)	-1813(2)	1709(2)	5614(2)	38(1)
C(202)	-1792(2)	937(2)	4771(2)	38(1)
C(203)	-1420(2)	173(2)	4792(2)	50(1)
C(204)	-1420(3)	-515(2)	3991(3)	62(1)
C(205)	-1829(3)	-471(2)	3143(2)	65(1)
C(206)	-2190(2)	286(2)	3112(2)	57(1)
C(207)	-2163(2)	994(2)	3922(2)	44(1)
C(208)	-2210(2)	1508(2)	6294(2)	48(1)
C(209)	-2978(3)	576(2)	5826(2)	60(1)
C(210)	-1301(3)	1527(2)	7091(2)	69(1)
C(211)	-2701(3)	2284(2)	6709(3)	77(1)
O(301)	-4119(4)	7497(4)	3147(4)	174(2)
C(301)	-4441(4)	8425(4)	3225(4)	114(2)
C(302)	-4948(6)	8411(4)	2298(4)	149(2)
C(303)	-3689(4)	7468(4)	4056(3)	114(2)
C(304)	-3356(3)	6538(3)	3954(3)	88(1)

Table 42. Bond lengths [A] and angles [deg] for **3a·4**$C_{11}H_{14}O\cdot Et_2O$ (pivalophenone).

Na(1)-O(1)	2.3156(16)	C(18)-C(23)	1.390(3)
Na(1)-O(3)#1	2.3187(16)	C(18)-C(19)	1.536(3)
Na(1)-O(101)	2.4339(18)	C(19)-C(21)	1.532(3)
Na(1)-O(2)	2.5875(16)	C(19)-C(20)	1.536(3)
Na(1)-C(17)	2.678(2)	C(19)-C(22)	1.540(3)
Na(1)-C(16)	2.942(2)	C(23)-C(24)	1.401(3)
Na(1)-Na(3)#1	3.1802(12)	C(24)-C(29)	1.385(3)
Na(1)-Na(2)#1	3.2619(12)	C(24)-C(25)	1.540(3)
Na(1)-Na(3)	4.1379(12)	C(25)-C(26)	1.527(4)
O(1)-C(3)	1.333(2)	C(25)-C(27)	1.535(4)
O(1)-Na(2)#1	2.3196(16)	C(25)-C(28)	1.536(4)
O(1)-Na(3)	2.3745(16)	C(30)-C(43)	1.396(3)
C(1)-C(16)	1.529(3)	C(30)-C(31)	1.421(3)
C(1)-C(30)	1.537(3)	C(31)-C(32)	1.433(3)
C(1)-C(2)	1.541(3)	C(32)-C(37)	1.387(3)
C(1)-Na(3)	2.984(2)	C(32)-C(33)	1.536(3)
Na(2)-O(1)#1	2.3196(16)	C(33)-C(36)	1.536(4)
Na(2)-O(2)	2.3439(16)	C(33)-C(34)	1.537(3)
Na(2)-O(201)	2.3944(19)	C(33)-C(35)	1.539(4)
Na(2)-O(3)	2.4426(16)	C(37)-C(38)	1.389(3)
Na(2)-C(31)	2.651(2)	C(38)-C(43)	1.387(3)
Na(2)-C(30)	2.898(2)	C(38)-C(39)	1.534(3)
Na(2)-Na(3)#1	3.1303(12)	C(39)-C(41)	1.523(3)
Na(2)-Na(1)#1	3.2619(12)	C(39)-C(40)	1.530(4)
Na(2)-Na(3)	4.0972(12)	C(39)-C(42)	1.535(4)
O(2)-C(17)	1.333(2)	O(101)-C(101)	1.225(3)
O(2)-Na(3)#1	2.2070(16)	C(101)-C(102)	1.496(4)
C(2)-C(15)	1.395(3)	C(101)-C(108)	1.535(3)
C(2)-C(3)	1.420(3)	C(102)-C(103)	1.391(4)
C(2)-Na(3)	2.830(2)	C(102)-C(107)	1.392(4)

Na(3)-O(2)#1	2.2070(16)	C(103)-C(104)	1.382(5)
Na(3)-O(3)	2.2499(16)	C(104)-C(105)	1.373(5)
Na(3)-C(3)	2.612(2)	C(105)-C(106)	1.380(5)
Na(3)-C(31)	3.074(2)	C(106)-C(107)	1.380(4)
Na(3)-Na(2)#1	3.1303(12)	C(108)-C(111)	1.510(5)
Na(3)-Na(1)#1	3.1802(12)	C(108)-C(109)	1.528(4)
O(3)-C(31)	1.339(2)	C(108)-C(110)	1.534(4)
O(3)-Na(1)#1	2.3187(15)	O(201)-C(201)	1.221(3)
C(3)-C(4)	1.439(3)	C(201)-C(202)	1.489(4)
C(4)-C(9)	1.390(3)	C(201)-C(208)	1.539(4)
C(4)-C(5)	1.537(3)	C(202)-C(203)	1.389(4)
C(5)-C(8)	1.535(3)	C(202)-C(207)	1.391(4)
C(5)-C(7)	1.535(3)	C(203)-C(204)	1.370(4)
C(5)-C(6)	1.543(3)	C(204)-C(205)	1.385(5)
C(9)-C(10)	1.393(3)	C(205)-C(206)	1.377(5)
C(10)-C(15)	1.384(3)	C(206)-C(207)	1.379(4)
C(10)-C(11)	1.539(3)	C(208)-C(209)	1.526(4)
C(11)-C(14)	1.527(4)	C(208)-C(211)	1.529(5)
C(11)-C(13)	1.528(4)	C(208)-C(210)	1.534(4)
C(11)-C(12)	1.528(4)	O(301)-C(303)	1.469(7)
C(16)-C(29)	1.393(3)	O(301)-C(301)	1.571(7)
C(16)-C(17)	1.422(3)	C(301)-C(302)	1.479(7)
C(17)-C(18)	1.433(3)	C(303)-C(304)	1.573(7)

O(1)-Na(1)-O(3)#1	92.61(6)	C(2)-Na(3)-Na(1)	57.90(4)
O(1)-Na(1)-O(101)	119.06(7)	C(1)-Na(3)-Na(1)	50.45(4)
O(3)#1-Na(1)-O(101)	123.02(7)	C(31)-Na(3)-Na(1)	93.72(4)
O(1)-Na(1)-O(2)	106.99(5)	Na(2)#1-Na(3)-Na(1)	51.06(2)
O(3)#1-Na(1)-O(2)	88.35(5)	Na(1)#1-Na(3)-Na(1)	98.95(3)
O(101)-Na(1)-O(2)	120.17(6)	Na(2)-Na(3)-Na(1)	65.86(2)
O(1)-Na(1)-C(17)	109.86(6)	C(31)-O(3)-Na(3)	115.49(12)
O(3)#1-Na(1)-C(17)	116.85(6)	C(31)-O(3)-Na(1)#1	156.09(13)
O(101)-Na(1)-C(17)	96.43(6)	Na(3)-O(3)-Na(1)#1	88.22(6)
O(2)-Na(1)-C(17)	29.27(5)	C(31)-O(3)-Na(2)	83.59(11)
O(1)-Na(1)-C(16)	85.40(6)	Na(3)-O(3)-Na(2)	121.60(6)
O(3)#1-Na(1)-C(16)	135.37(6)	Na(1)#1-O(3)-Na(2)	86.44(5)
O(101)-Na(1)-C(16)	95.89(6)	O(1)-C(3)-C(2)	120.09(17)
O(2)-Na(1)-C(16)	50.52(5)	O(1)-C(3)-C(4)	122.46(18)
C(17)-Na(1)-C(16)	28.83(6)	C(2)-C(3)-C(4)	117.38(17)
O(1)-Na(1)-Na(3)#1	106.60(5)	O(1)-C(3)-Na(3)	64.82(10)
O(3)#1-Na(1)-Na(3)#1	45.00(4)	C(2)-C(3)-Na(3)	83.55(11)
O(101)-Na(1)-Na(3)#1	133.98(6)	C(4)-C(3)-Na(3)	120.38(13)
O(2)-Na(1)-Na(3)#1	43.50(4)	C(9)-C(4)-C(3)	118.85(19)
C(17)-Na(1)-Na(3)#1	71.89(5)	C(9)-C(4)-C(5)	120.60(18)
C(16)-Na(1)-Na(3)#1	93.02(5)	C(3)-C(4)-C(5)	120.54(18)
O(1)-Na(1)-Na(2)#1	45.32(4)	C(8)-C(5)-C(7)	106.48(19)
O(3)#1-Na(1)-Na(2)#1	48.36(4)	C(8)-C(5)-C(4)	109.47(18)
O(101)-Na(1)-Na(2)#1	130.11(5)	C(7)-C(5)-C(4)	112.66(18)
O(2)-Na(1)-Na(2)#1	109.18(4)	C(8)-C(5)-C(6)	110.24(18)
C(17)-Na(1)-Na(2)#1	132.77(5)	C(7)-C(5)-C(6)	106.90(19)
C(16)-Na(1)-Na(2)#1	122.39(5)	C(4)-C(5)-C(6)	110.97(18)
Na(3)#1-Na(1)-Na(2)#1	78.98(3)	C(4)-C(9)-C(10)	123.96(19)
O(1)-Na(1)-Na(3)	28.47(4)	C(15)-C(10)-C(9)	116.62(19)
O(3)#1-Na(1)-Na(3)	83.23(4)	C(15)-C(10)-C(11)	121.88(19)
O(101)-Na(1)-Na(3)	144.65(6)	C(9)-C(10)-C(11)	121.50(19)
O(2)-Na(1)-Na(3)	79.89(4)	C(14)-C(11)-C(13)	109.2(2)
C(17)-Na(1)-Na(3)	90.32(5)	C(14)-C(11)-C(12)	107.9(2)
C(16)-Na(1)-Na(3)	74.12(4)	C(13)-C(11)-C(12)	108.1(3)
Na(3)#1-Na(1)-Na(3)	81.05(3)	C(14)-C(11)-C(10)	110.4(2)
Na(2)#1-Na(1)-Na(3)	48.28(2)	C(13)-C(11)-C(10)	109.40(19)
C(3)-O(1)-Na(1)	116.30(12)	C(12)-C(11)-C(10)	111.86(19)
C(3)-O(1)-Na(2)#1	153.98(13)	C(10)-C(15)-C(2)	122.65(19)
Na(1)-O(1)-Na(2)#1	89.45(5)	C(29)-C(16)-C(17)	120.25(18)

C(3)-O(1)-Na(3)	84.65(11)	C(29)-C(16)-C(1)	121.16(17)
Na(1)-O(1)-Na(3)	123.82(6)	C(17)-C(16)-C(1)	118.57(16)
Na(2)#1-O(1)-Na(3)	83.64(5)	C(29)-C(16)-Na(1)	119.76(14)
C(16)-C(1)-C(30)	112.86(16)	C(17)-C(16)-Na(1)	65.26(11)
C(16)-C(1)-C(2)	111.95(15)	C(1)-C(16)-Na(1)	85.63(11)
C(30)-C(1)-C(2)	111.61(15)	O(2)-C(17)-C(16)	119.56(17)
C(16)-C(1)-Na(3)	149.61(13)	O(2)-C(17)-C(18)	122.39(17)
C(30)-C(1)-Na(3)	93.23(11)	C(16)-C(17)-C(18)	118.02(17)
C(2)-C(1)-Na(3)	69.16(10)	O(2)-C(17)-Na(1)	71.58(10)
O(1)#1-Na(2)-O(2)	93.57(6)	C(16)-C(17)-Na(1)	85.91(12)
O(1)#1-Na(2)-O(201)	121.02(7)	C(18)-C(17)-Na(1)	111.18(13)
O(2)-Na(2)-O(201)	121.15(7)	C(23)-C(18)-C(17)	118.41(18)
O(1)#1-Na(2)-O(3)	89.40(5)	C(23)-C(18)-C(19)	120.77(18)
O(2)-Na(2)-O(3)	109.91(6)	C(17)-C(18)-C(19)	120.82(17)
O(201)-Na(2)-O(3)	115.82(6)	C(21)-C(19)-C(20)	106.90(19)
O(1)#1-Na(2)-C(31)	118.91(6)	C(21)-C(19)-C(18)	109.72(17)
O(2)-Na(2)-C(31)	110.83(6)	C(20)-C(19)-C(18)	112.69(18)
O(201)-Na(2)-C(31)	93.10(7)	C(21)-C(19)-C(22)	109.80(18)
O(3)-Na(2)-C(31)	30.12(5)	C(20)-C(19)-C(22)	107.22(19)
O(1)#1-Na(2)-C(30)	137.99(6)	C(18)-C(19)-C(22)	110.41(18)
O(2)-Na(2)-C(30)	85.60(6)	C(18)-C(23)-C(24)	124.17(19)
O(201)-Na(2)-C(30)	94.19(6)	C(29)-C(24)-C(23)	116.35(19)
O(3)-Na(2)-C(30)	52.38(5)	C(29)-C(24)-C(25)	123.1(2)
C(31)-Na(2)-C(30)	29.25(6)	C(23)-C(24)-C(25)	120.59(19)
O(1)#1-Na(2)-Na(3)#1	48.93(4)	C(26)-C(25)-C(27)	108.0(2)
O(2)-Na(2)-Na(3)#1	44.75(4)	C(26)-C(25)-C(28)	109.1(2)
O(201)-Na(2)-Na(3)#1	136.28(6)	C(27)-C(25)-C(28)	108.4(2)
O(3)-Na(2)-Na(3)#1	107.00(4)	C(26)-C(25)-C(24)	110.2(2)
C(31)-Na(2)-Na(3)#1	130.12(5)	C(27)-C(25)-C(24)	111.63(19)
C(30)-Na(2)-Na(3)#1	119.72(5)	C(28)-C(25)-C(24)	109.5(2)
O(1)#1-Na(2)-Na(1)#1	45.22(4)	C(24)-C(29)-C(16)	122.77(19)
O(2)-Na(2)-Na(1)#1	113.90(5)	C(43)-C(30)-C(31)	120.05(18)
O(201)-Na(2)-Na(1)#1	124.39(6)	C(43)-C(30)-C(1)	120.24(17)
O(3)-Na(2)-Na(1)#1	45.19(4)	C(31)-C(30)-C(1)	119.63(17)
C(31)-Na(2)-Na(1)#1	73.80(5)	C(43)-C(30)-Na(2)	122.70(13)
C(30)-Na(2)-Na(1)#1	97.25(5)	C(31)-C(30)-Na(2)	65.69(11)
Na(3)#1-Na(2)-Na(1)#1	80.65(3)	C(1)-C(30)-Na(2)	84.82(11)
O(1)#1-Na(2)-Na(3)	82.49(4)	O(3)-C(31)-C(30)	120.17(17)
O(2)-Na(2)-Na(3)	83.35(4)	O(3)-C(31)-C(32)	122.16(18)
O(201)-Na(2)-Na(3)	141.43(5)	C(30)-C(31)-C(32)	117.65(18)
O(3)-Na(2)-Na(3)	27.89(4)	O(3)-C(31)-Na(2)	66.29(10)
C(31)-Na(2)-Na(3)	48.59(5)	C(30)-C(31)-Na(2)	85.06(12)
C(30)-Na(2)-Na(3)	55.65(4)	C(32)-C(31)-Na(2)	118.15(14)
Na(3)#1-Na(2)-Na(3)	82.28(3)	O(3)-C(31)-Na(3)	41.36(9)
Na(1)#1-Na(2)-Na(3)	49.63(2)	C(30)-C(31)-Na(3)	92.09(12)
C(17)-O(2)-Na(3)#1	155.27(13)	C(32)-C(31)-Na(3)	138.42(14)
C(17)-O(2)-Na(2)	117.74(12)	Na(2)-C(31)-Na(3)	91.10(6)
Na(3)#1-O(2)-Na(2)	86.86(5)	C(37)-C(32)-C(31)	118.69(19)
C(17)-O(2)-Na(1)	79.15(11)	C(37)-C(32)-C(33)	120.85(19)
Na(3)#1-O(2)-Na(1)	82.70(5)	C(31)-C(32)-C(33)	120.46(18)
Na(2)-O(2)-Na(1)	130.34(6)	C(36)-C(33)-C(32)	109.9(2)
C(15)-C(2)-C(3)	120.49(18)	C(36)-C(33)-C(34)	106.7(2)
C(15)-C(2)-C(1)	119.66(17)	C(32)-C(33)-C(34)	112.4(2)
C(3)-C(2)-C(1)	119.81(17)	C(36)-C(33)-C(35)	110.8(2)
C(15)-C(2)-Na(3)	126.53(14)	C(32)-C(33)-C(35)	110.1(2)
C(3)-C(2)-Na(3)	66.53(10)	C(34)-C(33)-C(35)	107.1(2)
C(1)-C(2)-Na(3)	80.25(10)	C(32)-C(37)-C(38)	124.4(2)
O(2)#1-Na(3)-O(3)	100.40(6)	C(43)-C(38)-C(37)	116.22(18)
O(2)#1-Na(3)-O(1)	95.70(6)	C(43)-C(38)-C(39)	123.02(19)
O(3)-Na(3)-O(1)	121.30(6)	C(37)-C(38)-C(39)	120.75(19)
O(2)#1-Na(3)-C(3)	124.18(7)	C(41)-C(39)-C(40)	108.3(2)
O(3)-Na(3)-C(3)	118.41(6)	C(41)-C(39)-C(38)	112.43(19)
O(1)-Na(3)-C(3)	30.53(5)	C(40)-C(39)-C(38)	109.64(19)

O(2)#1-Na(3)-C(2)	148.12(6)	C(41)-C(39)-C(42)	107.5(2)
O(3)-Na(3)-C(2)	90.56(6)	C(40)-C(39)-C(42)	109.4(2)
O(1)-Na(3)-C(2)	53.71(5)	C(38)-C(39)-C(42)	109.56(19)
C(3)-Na(3)-C(2)	29.92(6)	C(38)-C(43)-C(30)	122.86(18)
O(2)#1-Na(3)-C(1)	133.21(6)	C(101)-O(101)-Na(1)	156.03(19)
O(3)-Na(3)-C(1)	64.65(5)	O(101)-C(101)-C(102)	118.9(2)
O(1)-Na(3)-C(1)	63.41(5)	O(101)-C(101)-C(108)	120.3(2)
C(3)-Na(3)-C(1)	54.01(6)	C(102)-C(101)-C(108)	120.8(2)
C(2)-Na(3)-C(1)	30.59(5)	C(103)-C(102)-C(107)	118.7(3)
O(2)#1-Na(3)-C(31)	123.54(6)	C(103)-C(102)-C(101)	117.0(2)
O(3)-Na(3)-C(31)	23.15(5)	C(107)-C(102)-C(101)	124.3(2)
O(1)-Na(3)-C(31)	113.03(6)	C(104)-C(103)-C(102)	120.2(3)
C(3)-Na(3)-C(31)	99.91(6)	C(105)-C(104)-C(103)	120.5(3)
C(2)-Na(3)-C(31)	70.33(6)	C(104)-C(105)-C(106)	119.9(3)
C(1)-Na(3)-C(31)	49.93(5)	C(107)-C(106)-C(105)	119.9(3)
O(2)#1-Na(3)-Na(2)#1	48.39(4)	C(106)-C(107)-C(102)	120.7(3)
O(3)-Na(3)-Na(2)#1	124.19(5)	C(111)-C(108)-C(109)	109.7(3)
O(1)-Na(3)-Na(2)#1	47.43(4)	C(111)-C(108)-C(110)	108.9(3)
C(3)-Na(3)-Na(2)#1	76.17(5)	C(109)-C(108)-C(110)	109.5(2)
C(2)-Na(3)-Na(2)#1	100.94(5)	C(111)-C(108)-C(101)	108.6(2)
C(1)-Na(3)-Na(2)#1	101.52(5)	C(109)-C(108)-C(101)	111.8(2)
C(31)-Na(3)-Na(2)#1	137.30(5)	C(110)-C(108)-C(101)	108.3(2)
O(2)#1-Na(3)-Na(1)#1	53.80(4)	C(201)-O(201)-Na(2)	152.64(19)
O(3)-Na(3)-Na(1)#1	46.78(4)	O(201)-C(201)-C(202)	119.0(2)
O(1)-Na(3)-Na(1)#1	123.35(5)	O(201)-C(201)-C(208)	120.1(2)
C(3)-Na(3)-Na(1)#1	147.14(5)	C(202)-C(201)-C(208)	120.9(2)
C(2)-Na(3)-Na(1)#1	131.76(5)	C(203)-C(202)-C(207)	118.9(3)
C(1)-Na(3)-Na(1)#1	101.30(5)	C(203)-C(202)-C(201)	123.5(2)
C(31)-Na(3)-Na(1)#1	69.90(4)	C(207)-C(202)-C(201)	117.6(2)
Na(2)#1-Na(3)-Na(1)#1	90.37(3)	C(204)-C(203)-C(202)	120.8(3)
O(2)#1-Na(3)-Na(2)	93.87(5)	C(203)-C(204)-C(205)	119.9(3)
O(3)-Na(3)-Na(2)	30.52(4)	C(206)-C(205)-C(204)	120.0(3)
O(1)-Na(3)-Na(2)	92.83(4)	C(205)-C(206)-C(207)	120.2(3)
C(3)-Na(3)-Na(2)	100.21(5)	C(206)-C(207)-C(202)	120.2(3)
C(2)-Na(3)-Na(2)	80.52(4)	C(209)-C(208)-C(211)	109.0(3)
C(1)-Na(3)-Na(2)	49.95(4)	C(209)-C(208)-C(210)	109.9(2)
C(31)-Na(3)-Na(2)	40.31(4)	C(211)-C(208)-C(210)	108.4(3)
Na(2)#1-Na(3)-Na(2)	97.72(3)	C(209)-C(208)-C(201)	113.1(2)
Na(1)#1-Na(3)-Na(2)	51.39(2)	C(211)-C(208)-C(201)	108.5(2)
O(2)#1-Na(3)-Na(1)	91.05(4)	C(210)-C(208)-C(201)	107.7(2)
O(3)-Na(3)-Na(1)	95.65(4)	C(303)-O(301)-C(301)	113.3(5)
O(1)-Na(3)-Na(1)	27.70(4)	C(302)-C(301)-O(301)	112.5(4)
C(3)-Na(3)-Na(1)	49.39(5)	O(301)-C(303)-C(304)	111.9(4)

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

Table 43. Anisotropic displacement parameters (A^2 x 10^3) for **3a·4$C_{11}H_{14}O$·Et_2O** (pivalophenone). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Na(1)	26(1)	26(1)	24(1)	9(1)	8(1)	5(1)
Na(2)	25(1)	25(1)	26(1)	11(1)	8(1)	5(1)
Na(3)	27(1)	26(1)	20(1)	8(1)	7(1)	2(1)
O(1)	20(1)	26(1)	20(1)	10(1)	5(1)	4(1)
O(2)	22(1)	21(1)	20(1)	6(1)	3(1)	4(1)
O(3)	22(1)	24(1)	21(1)	7(1)	6(1)	1(1)

C(1)	19(1)	21(1)	17(1)	8(1)	5(1)	4(1)
C(2)	22(1)	22(1)	17(1)	8(1)	7(1)	7(1)
C(3)	21(1)	23(1)	17(1)	7(1)	7(1)	6(1)
C(4)	25(1)	28(1)	20(1)	11(1)	8(1)	6(1)
C(5)	29(1)	31(1)	28(1)	17(1)	8(1)	5(1)
C(6)	37(1)	33(1)	31(1)	14(1)	17(1)	3(1)
C(7)	44(1)	49(2)	47(2)	36(1)	10(1)	5(1)
C(8)	35(1)	28(1)	37(1)	16(1)	14(1)	7(1)
C(9)	28(1)	36(1)	24(1)	20(1)	7(1)	11(1)
C(10)	21(1)	35(1)	24(1)	15(1)	6(1)	9(1)
C(11)	21(1)	47(1)	37(1)	25(1)	4(1)	9(1)
C(12)	22(1)	84(2)	88(2)	59(2)	-2(1)	-3(1)
C(13)	32(1)	86(2)	36(2)	15(2)	-4(1)	8(1)
C(14)	33(1)	70(2)	58(2)	34(2)	10(1)	21(1)
C(15)	22(1)	27(1)	25(1)	12(1)	8(1)	5(1)
C(16)	21(1)	22(1)	18(1)	9(1)	8(1)	5(1)
C(17)	23(1)	21(1)	19(1)	10(1)	8(1)	3(1)
C(18)	25(1)	22(1)	24(1)	11(1)	9(1)	6(1)
C(19)	29(1)	24(1)	26(1)	9(1)	7(1)	10(1)
C(20)	42(1)	34(1)	41(1)	10(1)	9(1)	19(1)
C(21)	29(1)	37(1)	34(1)	13(1)	12(1)	12(1)
C(22)	38(1)	31(1)	37(1)	20(1)	9(1)	11(1)
C(23)	33(1)	23(1)	24(1)	5(1)	11(1)	8(1)
C(24)	28(1)	28(1)	20(1)	6(1)	7(1)	4(1)
C(25)	34(1)	34(1)	21(1)	0(1)	3(1)	6(1)
C(26)	56(2)	40(2)	35(1)	1(1)	1(1)	-7(1)
C(27)	41(2)	58(2)	28(1)	-5(1)	-5(1)	13(1)
C(28)	52(2)	53(2)	25(1)	3(1)	12(1)	11(1)
C(29)	23(1)	28(1)	20(1)	9(1)	6(1)	6(1)
C(30)	20(1)	21(1)	22(1)	12(1)	7(1)	7(1)
C(31)	22(1)	22(1)	22(1)	11(1)	7(1)	5(1)
C(32)	28(1)	26(1)	26(1)	9(1)	13(1)	5(1)
C(33)	45(1)	32(1)	35(1)	4(1)	27(1)	0(1)
C(34)	72(2)	54(2)	58(2)	-6(1)	52(2)	-10(2)
C(35)	68(2)	43(2)	26(1)	7(1)	19(1)	-5(1)
C(36)	56(2)	34(1)	58(2)	4(1)	35(2)	11(1)
C(37)	28(1)	30(1)	35(1)	13(1)	18(1)	4(1)
C(38)	23(1)	23(1)	27(1)	9(1)	7(1)	2(1)
C(39)	27(1)	27(1)	34(1)	8(1)	10(1)	-2(1)
C(40)	27(1)	49(2)	79(2)	9(2)	12(1)	1(1)
C(41)	39(1)	35(1)	38(1)	2(1)	10(1)	-10(1)
C(42)	64(2)	36(1)	49(2)	13(1)	22(1)	-13(1)
C(43)	25(1)	22(1)	18(1)	7(1)	7(1)	5(1)
O(101)	54(1)	44(1)	28(1)	7(1)	20(1)	3(1)
C(101)	38(1)	36(1)	30(1)	5(1)	16(1)	-2(1)
C(102)	40(1)	35(1)	33(1)	4(1)	18(1)	2(1)
C(103)	45(2)	43(2)	51(2)	2(1)	25(1)	1(1)
C(104)	42(2)	58(2)	73(2)	1(2)	23(2)	9(1)
C(105)	59(2)	64(2)	59(2)	4(2)	5(2)	27(2)
C(106)	80(2)	60(2)	47(2)	19(2)	23(2)	30(2)
C(107)	54(2)	52(2)	40(2)	17(1)	25(1)	16(1)
C(108)	43(2)	59(2)	28(1)	11(1)	15(1)	15(1)
C(109)	60(2)	61(2)	39(2)	3(1)	21(1)	21(2)
C(110)	41(2)	104(3)	55(2)	10(2)	24(2)	13(2)
C(111)	134(4)	107(3)	54(2)	35(2)	43(2)	82(3)
O(201)	44(1)	35(1)	57(1)	26(1)	12(1)	3(1)
C(201)	34(1)	34(1)	44(1)	23(1)	6(1)	2(1)
C(202)	34(1)	37(1)	46(1)	25(1)	12(1)	5(1)
C(203)	59(2)	44(2)	59(2)	33(1)	22(2)	16(1)
C(204)	78(2)	43(2)	79(2)	30(2)	41(2)	20(2)
C(205)	70(2)	55(2)	62(2)	13(2)	35(2)	5(2)
C(206)	53(2)	70(2)	50(2)	30(2)	20(1)	7(2)
C(207)	38(1)	50(2)	49(2)	31(1)	12(1)	8(1)

C(208)	58(2)	39(1)	41(1)	18(1)	13(1)	-2(1)
C(209)	68(2)	56(2)	54(2)	26(2)	22(2)	-7(2)
C(210)	84(2)	58(2)	48(2)	33(2)	0(2)	-12(2)
C(211)	105(3)	64(2)	75(2)	28(2)	54(2)	21(2)
O(301)	194(5)	162(4)	140(4)	35(3)	75(4)	28(4)
C(301)	106(4)	85(3)	104(4)	0(3)	35(3)	12(3)
C(302)	197(7)	102(4)	99(4)	15(3)	33(4)	24(4)
C(303)	80(3)	153(5)	58(3)	9(3)	18(2)	-4(3)
C(304)	63(2)	115(4)	66(2)	20(2)	30(2)	-2(2)

Table 44. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3a**·4$C_{11}H_{14}O$·Et_2O (pivalophenone).

	x	y	z	U(eq)
H(1A)	-1255	4130	3994	24
H(6A)	-101	6344	2021	49
H(6B)	-747	5320	1392	49
H(6C)	-128	5640	2460	49
H(7A)	-2569	6636	1619	66
H(7B)	-2255	5900	878	66
H(7C)	-1569	6911	1491	66
H(8A)	-1646	7197	3277	49
H(8B)	-626	7462	3175	49
H(8C)	-724	6820	3669	49
H(9A)	-3373	5262	1292	33
H(12A)	-6150	3081	850	97
H(12B)	-5389	3537	1896	97
H(12C)	-5172	2728	1134	97
H(13A)	-5672	3331	-361	90
H(13B)	-4707	2967	-61	90
H(13C)	-4605	3938	-85	90
H(14A)	-6080	4565	803	79
H(14B)	-5053	5229	1063	79
H(14C)	-5321	5080	1848	79
H(15A)	-3753	3491	2364	29
H(20A)	645	641	2099	64
H(20B)	99	136	2526	64
H(20C)	1276	503	2973	64
H(21A)	1426	2333	2963	51
H(21B)	2066	2136	3793	51
H(21C)	1441	2891	3971	51
H(22A)	1220	1376	4513	53
H(22B)	45	1002	4085	53
H(22C)	525	2073	4654	53
H(23A)	-941	679	1644	34
H(26A)	-3436	-675	-161	82
H(26B)	-3427	-193	856	82
H(26C)	-2450	-452	705	82
H(27A)	-4088	584	-454	82
H(27B)	-3473	1621	153	82
H(27C)	-4015	1112	580	82
H(28A)	-2574	169	-774	73
H(28B)	-1546	412	56	73
H(28C)	-1964	1206	-152	73
H(29A)	-2802	2371	1735	29
H(34A)	-4645	4444	5969	99

H(34B)	-3961	4944	7039	99
H(34C)	-4049	3888	6458	99
H(35A)	-1590	4945	6848	74
H(35B)	-2205	4176	6971	74
H(35C)	-2123	5228	7567	74
H(36A)	-3744	5666	5746	76
H(36B)	-2566	5893	6075	76
H(36C)	-3070	6138	6818	76
H(37A)	-4481	3164	4938	36
H(40A)	-6033	2353	2724	91
H(40B)	-6028	2424	3689	91
H(40C)	-6555	1487	2781	91
H(41A)	-5030	1385	1962	67
H(41B)	-5560	537	2040	67
H(41C)	-4380	855	2448	67
H(42A)	-5522	627	3527	80
H(42B)	-5011	1551	4451	80
H(42C)	-4344	976	3985	80
H(43A)	-3450	2297	2888	27
H(10A)	-1562	3070	1006	61
H(10B)	-2910	3456	157	80
H(10C)	-2757	4016	-886	86
H(10D)	-1246	4193	-1090	76
H(10E)	79	3733	-309	57
H(10F)	627	1385	-770	88
H(10G)	29	2132	-873	88
H(10H)	-360	1412	-558	88
H(11A)	2117	2755	235	110
H(11B)	2164	3490	1202	110
H(11C)	1480	3501	269	110
H(11D)	1685	1555	771	138
H(11E)	719	1492	1012	138
H(11F)	1661	2329	1683	138
H(20D)	-1167	130	5356	60
H(20E)	-1147	-1012	4017	75
H(20F)	-1858	-952	2594	78
H(20G)	-2454	320	2544	69
H(20H)	-2393	1511	3900	53
H(20I)	-3231	505	6270	90
H(20J)	-2660	81	5607	90
H(20K)	-3526	554	5305	90
H(21D)	-1528	1401	7526	103
H(21E)	-842	2129	7409	103
H(21F)	-964	1063	6838	103
H(21G)	-2937	2176	7146	115
H(21H)	-3259	2294	6215	115
H(21I)	-2214	2871	7025	115
H(30A)	-4893	8529	3560	137
H(30B)	-3847	8939	3584	137
H(30C)	-5206	8955	2377	223
H(30D)	-5494	7866	1915	223
H(30F)	-4472	8402	2001	223
H(30E)	-4187	7529	4343	137
H(30H)	-3110	7990	4467	137
H(30G)	-3143	6518	4551	133
H(30I)	-2807	6511	3742	133
H(30J)	-3914	6019	3509	133

Table 45. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3a·5.6$C_8H_{14}O$** (2,6-dimethyl cyclohexanone).
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)	Site Occupancy
Na(1)	4297(1)	5620(1)	5546(1)	33(1)	
O(1)	5095(1)	5998(1)	5264(1)	30(1)	
C(1)	4500(2)	5807(2)	4127(2)	27(1)	
Na(2)	4493(1)	4575(1)	4070(1)	34(1)	
O(2)	3993(1)	4981(1)	4802(1)	29(1)	
C(2)	4751(2)	6346(2)	4301(2)	31(1)	
Na(3)	5691(1)	5642(1)	4521(1)	32(1)	
O(3)	5305(1)	5031(1)	3860(1)	28(1)	
C(3)	5019(2)	6411(2)	4888(2)	31(1)	
C(4)	5220(2)	6929(2)	5046(2)	38(1)	
C(5)	5522(2)	7030(2)	5671(2)	45(1)	
C(6)	5171(2)	6897(2)	6216(2)	59(1)	
C(7)	5681(3)	7621(2)	5751(3)	69(2)	
C(8)	6043(2)	6709(2)	5701(3)	56(1)	
C(9)	5131(2)	7333(2)	4623(2)	44(1)	
C(10)	4877(2)	7273(2)	4047(2)	46(1)	
C(11)	4783(2)	7749(2)	3608(3)	61(2)	
C(12A)	5325(5)	8019(5)	3477(8)	112(5)	0.5
C(12B)	4915(19)	8284(8)	3946(12)	113(13)	0.5
C(13A)	4513(7)	7576(4)	2968(6)	112(4)	0.5
C(13B)	5098(11)	7695(9)	3075(11)	73(7)	0.5
C(14A)	4441(7)	8148(5)	3927(7)	103(5)	0.5
C(14B)	4143(10)	7753(13)	3390(20)	123(14)	0.5
C(15)	4701(2)	6774(2)	3896(2)	37(1)	
C(16)	3887(2)	5786(2)	4238(2)	28(1)	
C(17)	3668(2)	5352(2)	4556(2)	30(1)	
C(18)	3097(2)	5331(2)	4626(2)	35(1)	
C(19)	2833(2)	4875(2)	4979(2)	47(1)	
C(20)	3029(2)	4883(2)	5658(2)	56(1)	
C(21)	2965(2)	4344(2)	4685(3)	62(2)	
C(22)	2216(2)	4921(3)	4971(3)	76(2)	
C(23)	2785(2)	5738(2)	4373(2)	39(1)	
C(24)	2996(2)	6174(2)	4064(2)	37(1)	
C(25)	2618(2)	6594(2)	3773(2)	45(1)	
C(26)	2311(3)	6350(3)	3223(3)	83(2)	
C(27)	2225(3)	6798(3)	4237(3)	76(2)	
C(28)	2926(3)	7060(3)	3522(4)	83(2)	
C(29)	3548(2)	6190(2)	4014(2)	34(1)	
C(30)	4635(2)	5627(2)	3463(2)	28(1)	
C(31)	5055(2)	5256(2)	3369(2)	28(1)	
C(32)	5179(2)	5121(2)	2747(2)	32(1)	
C(33)	5610(2)	4699(2)	2606(2)	43(1)	
C(34)	5677(3)	4622(3)	1907(2)	69(2)	
C(35)	5428(2)	4161(2)	2868(2)	57(1)	
C(36)	6162(2)	4850(2)	2896(2)	55(1)	
C(37)	4892(2)	5361(2)	2264(2)	37(1)	
C(38)	4470(2)	5719(2)	2350(2)	38(1)	
C(39)	4169(2)	5963(2)	1789(2)	51(1)	
C(40)	3954(3)	5525(3)	1352(3)	74(2)	
C(41)	3693(2)	6299(3)	1979(2)	61(2)	

C(42)	4562(3)	6322(3)	1443(3)	78(2)	
C(43)	4350(2)	5831(2)	2952(2)	35(1)	
O(101)	3694(2)	6239(2)	5868(2)	77(1)	
C(101)	3381(2)	6571(2)	6005(3)	64(2)	
C(102)	2967(3)	6458(3)	6498(5)	105(3)	
C(103)	2983(6)	6843(4)	6982(6)	173(6)	
C(104)	2891(4)	7415(4)	6665(5)	133(3)	
C(105)	3345(4)	7502(4)	6215(5)	133(3)	
C(106)	3353(3)	7114(3)	5735(3)	80(2)	
C(107)	2385(3)	6391(5)	6147(6)	168(5)	
C(108)	3769(3)	7225(3)	5265(3)	79(2)	
O(201)	3937(3)	4432(2)	3223(3)	122(2)	
C(201)	3619(3)	4353(4)	2850(5)	103(3)	
C(202)	3784(7)	3866(7)	2452(8)	207(6)	
C(203)	3406(6)	3423(5)	2372(7)	179(5)	
C(204)	2906(8)	3700(7)	2228(9)	214(7)	
C(205)	2678(6)	4153(6)	2598(8)	195(6)	
C(206)	3088(5)	4554(5)	2606(6)	149(4)	
C(207)	4016(6)	4071(6)	1834(7)	192(5)	
C(208)	2899(5)	5022(4)	2933(5)	139(4)	
O(301)	6165(2)	6279(2)	4000(2)	87(2)	
C(301)	6327(2)	6521(2)	3579(3)	66(2)	
C(302)	6623(5)	7000(4)	3560(7)	172(6)	
C(303)	7184(5)	6893(5)	3221(7)	186(7)	
C(304)	6969(6)	6700(4)	2578(5)	147(4)	
C(305)	6724(4)	6198(5)	2599(6)	155(5)	
C(306)	6170(5)	6275(5)	2959(6)	141(4)	
C(307)	6715(5)	7293(4)	4166(5)	141(4)	
C(308)	5766(3)	6520(4)	2609(5)	119(3)	
Na(1B)	-960(1)	9611(1)	-5134(1)	32(1)	
O(1B)	-471(1)	9363(1)	-4263(1)	28(1)	
C(1B)	-786(2)	10441(2)	-4087(2)	26(1)	
Na(2B)	-120(1)	11021(1)	-5092(1)	33(1)	
O(2B)	-831(1)	10509(1)	-5412(1)	29(1)	
C(2B)	-862(2)	10005(2)	-3598(2)	30(1)	
Na(3B)	298(1)	9826(1)	-3850(1)	34(1)	
O(3B)	340(1)	10681(1)	-4196(1)	30(1)	
C(3B)	-711(2)	9474(2)	-3734(2)	29(1)	
C(4B)	-803(2)	9078(2)	-3274(2)	37(1)	
C(5B)	-618(2)	8499(2)	-3373(2)	51(1)	
C(6B)	-887(2)	8260(2)	-3953(3)	64(2)	
C(7B)	-764(3)	8135(2)	-2827(3)	81(2)	
C(8B)	-4(2)	8480(2)	-3415(3)	60(2)	
C(9B)	-1044(2)	9226(2)	-2734(2)	49(1)	
C(10B)	-1191(2)	9740(2)	-2593(2)	48(1)	
C(11B)	-1470(3)	9875(3)	-1987(3)	73(2)	
C(12C)	-1947(7)	9517(9)	-1939(9)	109(7)	0.6
C(12D)	-2070(7)	10043(10)	-2148(8)	111(6)	0.4
C(13C)	-1566(8)	10443(7)	-1903(7)	85(5)	0.6
C(13D)	-1225(9)	10343(8)	-1675(7)	102(6)	0.4
C(14C)	-1081(7)	9645(7)	-1420(5)	87(5)	0.6
C(14D)	-1511(11)	9416(9)	-1566(11)	135(7)	0.4
C(15B)	-1087(2)	10120(2)	-3033(2)	38(1)	
C(16B)	-1301(2)	10571(1)	-4465(2)	26(1)	
C(17B)	-1285(2)	10618(2)	-5122(2)	28(1)	
C(18B)	-1769(2)	10772(2)	-5457(2)	33(1)	
C(19B)	-1786(2)	10823(2)	-6167(2)	44(1)	
C(20B)	-1675(2)	10278(2)	-6460(2)	54(1)	
C(21B)	-1388(2)	11232(2)	-6381(3)	58(1)	
C(22B)	-2347(2)	10994(3)	-6423(3)	63(2)	
C(23B)	-2225(2)	10870(2)	-5124(2)	40(1)	
C(24B)	-2252(2)	10821(2)	-4485(2)	37(1)	
C(25B)	-2771(2)	10972(2)	-4158(3)	53(1)	

C(26B)	-3250(2)	10671(3)	-4424(3)	80(2)	
C(27B)	-2730(2)	10868(3)	-3456(3)	88(2)	
C(28B)	-2860(3)	11569(3)	-4248(5)	111(3)	
C(29B)	-1782(2)	10661(2)	-4168(2)	34(1)	
C(30B)	-508(2)	10941(2)	-3808(2)	27(1)	
C(31B)	53(2)	11015(2)	-3861(2)	26(1)	
C(32B)	294(2)	11469(2)	-3573(2)	35(1)	
C(33B)	903(2)	11585(2)	-3630(3)	48(1)	
C(34B)	1023(2)	11697(2)	-4306(3)	57(1)	
C(35B)	1244(2)	11124(2)	-3391(3)	66(2)	
C(36B)	1079(2)	12081(2)	-3255(3)	73(2)	
C(37B)	-33(2)	11808(2)	-3242(2)	36(1)	
C(38B)	-584(2)	11745(2)	-3196(2)	34(1)	
C(39B)	-916(2)	12133(2)	-2805(2)	41(1)	
C(40B)	-1520(2)	12029(2)	-2872(3)	65(2)	
C(41B)	-737(3)	12088(2)	-2129(3)	67(2)	
C(42B)	-817(2)	12712(2)	-3011(3)	61(2)	
C(43B)	-813(2)	11313(2)	-3490(2)	30(1)	
O(401)	-1851(2)	9383(2)	-5117(3)	85(2)	
C(401)	-2228(2)	9226(2)	-4869(3)	64(2)	
C(402)	-2792(3)	9236(4)	-5102(5)	117(3)	
C(403)	-2968(4)	8631(4)	-5167(7)	156(5)	
C(404)	-2911(4)	8418(4)	-4525(6)	128(4)	
C(405)	-2339(5)	8414(4)	-4283(6)	146(4)	
C(406)	-2126(4)	8987(4)	-4225(5)	121(3)	
C(407)	-2895(4)	9540(4)	-5687(5)	116(3)	
C(408)	-2314(4)	9281(4)	-3711(4)	113(3)	
O(501)	-296(2)	11911(2)	-5049(2)	90(2)	
C(501)	-424(3)	12366(3)	-4975(3)	74(2)	
C(502)	-19(3)	12811(3)	-4997(4)	87(2)	
C(503)	-198(4)	13212(3)	-5503(4)	108(3)	
C(504)	-783(4)	13395(3)	-5421(5)	112(3)	
C(505)	-1146(4)	12929(3)	-5415(4)	99(2)	
C(506)	-993(3)	12531(3)	-4912(3)	75(2)	
C(507)	78(4)	13070(4)	-4360(4)	114(3)	
C(508)	-1378(3)	12063(3)	-4872(4)	95(2)	
O(601)	419(2)	9812(3)	-2779(2)	63(2)	0.6
C(601)	486(3)	9929(3)	-2267(4)	51(2)	0.6
C(602)	595(7)	9626(5)	-1713(7)	149(7)	0.6
C(603)	1024(8)	9791(6)	-1264(9)	183(10)	0.6
C(604)	960(10)	10392(8)	-1172(9)	224(12)	0.6
C(605)	1003(10)	10674(7)	-1778(10)	233(12)	0.6
C(606)	536(6)	10530(5)	-2235(8)	143(6)	0.6
C(607)	559(7)	9085(6)	-1746(9)	145(6)	0.6
C(608)	58(5)	10791(4)	-2061(5)	88(4)	0.6
O(801)	4880(6)	4988(7)	-159(7)	106(4)	0.4
C(801)	5495(12)	5794(11)	-19(14)	121(9)	0.4
C(802)	5431(8)	5322(7)	170(9)	75(4)	0.4
O(803)	5661(13)	5731(13)	247(16)	143(11)	0.4
C(804)	5132(9)	5488(9)	-73(11)	105(6)	0.4
C(901)	-2426(19)	7170(20)	-3610(30)	138(19)	0.2
C(902)	-2106(18)	7132(16)	-3330(15)	150(14)	0.3
O(901)	-1725(15)	6825(15)	-4146(14)	165(13)	0.25
C(904)	-1512(18)	6673(18)	-5092(19)	125(13)	0.25
C(905)	-1512(14)	6620(14)	-4554(15)	91(10)	0.25
C(906)	-1777(11)	6935(11)	-3627(14)	74(7)	0.25
C(907)	-1618(17)	6767(19)	-4776(16)	117(13)	0.25
C(908)	-1655(12)	6746(11)	-5421(12)	78(7)	0.25
O(902)	-1921(10)	6970(9)	-4450(12)	105(7)	0.25
C(909)	-1994(19)	6956(19)	-3921(15)	134(15)	0.25

Table 46. Bond lengths [A] and angles [deg] for **3a·5.6$C_8H_{14}O$** 2,6-dimethyl cyclohexanone).

Na(1)-O(3)#1	2.290(3)	C(11)-C(14B)	1.64(3)
Na(1)-O(101)	2.291(4)	C(16)-C(29)	1.402(6)
Na(1)-O(1)	2.302(3)	C(16)-C(17)	1.413(6)
Na(1)-O(2)	2.386(3)	C(17)-C(18)	1.432(6)
Na(1)-C(17)	2.694(4)	C(18)-C(23)	1.392(6)
Na(1)-C(16)	3.001(4)	C(18)-C(19)	1.543(6)
Na(1)-C(3)	3.067(4)	C(19)-C(21)	1.527(8)
Na(1)-Na(2)#1	3.133(2)	C(19)-C(20)	1.528(7)
Na(1)-Na(3)#1	3.196(2)	C(19)-C(22)	1.536(7)
Na(1)-Na(3)	4.169(2)	C(23)-C(24)	1.401(6)
Na(1)-Na(2)	4.181(2)	C(24)-C(29)	1.377(6)
O(1)-C(3)	1.333(5)	C(24)-C(25)	1.539(6)
O(1)-Na(2)#1	2.264(3)	C(25)-C(27)	1.513(7)
O(1)-Na(3)	2.393(3)	C(25)-C(28)	1.514(8)
C(1)-C(2)	1.543(6)	C(25)-C(26)	1.526(8)
C(1)-C(30)	1.548(5)	C(30)-C(43)	1.391(6)
C(1)-C(16)	1.551(5)	C(30)-C(31)	1.425(5)
C(1)-Na(3)	3.079(4)	C(31)-C(32)	1.430(6)
C(1)-Na(2)	3.117(4)	C(32)-C(37)	1.385(6)
Na(2)-O(1)#1	2.264(3)	C(32)-C(33)	1.548(6)
Na(2)-O(201)	2.284(5)	C(33)-C(34)	1.534(7)
Na(2)-O(2)	2.285(3)	C(33)-C(36)	1.538(7)
Na(2)-O(3)	2.379(3)	C(33)-C(35)	1.546(7)
Na(2)-C(31)	2.709(4)	C(37)-C(38)	1.401(6)
Na(2)-C(30)	2.993(4)	C(38)-C(43)	1.373(6)
Na(2)-C(17)	3.050(4)	C(38)-C(39)	1.531(6)
Na(2)-Na(1)#1	3.133(2)	C(39)-C(41)	1.524(7)
Na(2)-Na(3)#1	3.140(2)	C(39)-C(40)	1.535(8)
Na(2)-Na(3)	4.112(2)	C(39)-C(42)	1.544(8)
O(2)-C(17)	1.336(5)	O(101)-C(101)	1.188(6)
O(2)-Na(3)#1	2.274(3)	C(101)-C(106)	1.491(9)
C(2)-C(15)	1.393(6)	C(101)-C(102)	1.532(9)
C(2)-C(3)	1.423(6)	C(102)-C(103)	1.425(14)
C(2)-Na(3)	2.964(4)	C(102)-C(107)	1.624(13)
Na(3)-O(2)#1	2.274(3)	C(103)-C(104)	1.605(15)
Na(3)-O(3)	2.293(3)	C(104)-C(105)	1.530(14)
Na(3)-O(301)	2.309(4)	C(105)-C(106)	1.427(12)
Na(3)-C(3)	2.699(4)	C(106)-C(108)	1.499(10)
Na(3)-C(31)	3.063(4)	O(201)-C(201)	1.136(9)
Na(3)-Na(2)#1	3.140(2)	C(201)-C(206)	1.458(14)
Na(3)-Na(1)#1	3.196(2)	C(201)-C(202)	1.570(18)
O(3)-C(31)	1.339(5)	C(202)-C(203)	1.492(18)
O(3)-Na(1)#1	2.290(3)	C(202)-C(207)	1.54(2)
C(3)-C(4)	1.439(6)	C(203)-C(204)	1.453(18)
C(4)-C(9)	1.387(7)	C(204)-C(205)	1.556(19)
C(4)-C(5)	1.545(7)	C(205)-C(206)	1.382(19)
C(5)-C(6)	1.529(7)	C(206)-C(208)	1.57(2)
C(5)-C(8)	1.531(7)	O(301)-C(301)	1.178(7)
C(5)-C(7)	1.552(7)	C(301)-C(302)	1.413(10)
C(9)-C(10)	1.384(7)	C(301)-C(306)	1.519(13)
C(10)-C(15)	1.372(7)	C(302)-C(307)	1.523(14)
C(10)-C(11)	1.546(6)	C(302)-C(303)	1.621(14)
C(11)-C(13B)	1.42(2)	C(303)-C(304)	1.548(17)
C(11)-C(14A)	1.509(12)	C(304)-C(305)	1.396(14)
C(11)-C(12A)	1.549(12)	C(305)-C(306)	1.607(14)
C(11)-C(12B)	1.58(3)	C(306)-C(308)	1.373(13)
C(11)-C(13A)	1.585(14)		
Na(1B)-O(3B)#2	2.269(3)	C(11B)-C(14C)	1.642(14)

Na(1B)-O(401)	2.288(4)	C(16B)-C(29B)	1.393(6)
Na(1B)-O(1B)	2.293(3)	C(16B)-C(17B)	1.425(6)
Na(1B)-O(2B)	2.375(3)	C(17B)-C(18B)	1.440(6)
Na(1B)-C(17B)	2.676(4)	C(18B)-C(23B)	1.382(6)
Na(1B)-C(16B)	2.963(4)	C(18B)-C(19B)	1.536(6)
Na(1B)-C(3B)	3.085(4)	C(19B)-C(21B)	1.516(7)
Na(1B)-C(1B)	3.107(4)	C(19B)-C(20B)	1.543(7)
Na(1B)-Na(3B)#2	3.127(2)	C(19B)-C(22B)	1.547(6)
Na(1B)-Na(2B)#2	3.148(2)	C(23B)-C(24B)	1.390(7)
Na(1B)-Na(2B)	4.131(2)	C(24B)-C(29B)	1.394(6)
Na(1B)-Na(3B)	4.146(2)	C(24B)-C(25B)	1.540(6)
O(1B)-C(3B)	1.335(5)	C(25B)-C(26B)	1.512(7)
O(1B)-Na(2B)#2	2.273(3)	C(25B)-C(28B)	1.535(9)
O(1B)-Na(3B)	2.388(3)	C(25B)-C(27B)	1.542(9)
C(1B)-C(16B)	1.530(5)	C(30B)-C(43B)	1.403(5)
C(1B)-C(2B)	1.542(5)	C(30B)-C(31B)	1.414(5)
C(1B)-C(30B)	1.553(5)	C(31B)-C(32B)	1.428(6)
Na(2B)-O(1B)#2	2.273(3)	C(32B)-C(37B)	1.395(6)
Na(2B)-O(2B)	2.278(3)	C(32B)-C(33B)	1.548(6)
Na(2B)-O(501)	2.297(4)	C(33B)-C(35B)	1.523(7)
Na(2B)-O(3B)	2.380(3)	C(33B)-C(34B)	1.525(8)
Na(2B)-C(31B)	2.680(4)	C(33B)-C(36B)	1.550(6)
Na(2B)-C(30B)	2.971(4)	C(37B)-C(38B)	1.384(6)
Na(2B)-C(17B)	3.066(4)	C(38B)-C(43B)	1.378(6)
Na(2B)-Na(1B)#2	3.148(2)	C(38B)-C(39B)	1.549(6)
Na(2B)-Na(3B)#2	3.151(2)	C(39B)-C(41B)	1.516(7)
Na(2B)-Na(3B)	4.152(2)	C(39B)-C(40B)	1.526(7)
O(2B)-C(17B)	1.337(5)	C(39B)-C(42B)	1.553(7)
O(2B)-Na(3B)#2	2.269(3)	O(401)-C(401)	1.166(6)
C(2B)-C(15B)	1.387(6)	C(401)-C(402)	1.471(10)
C(2B)-C(3B)	1.429(6)	C(401)-C(406)	1.533(11)
C(2B)-Na(3B)	2.984(4)	C(402)-C(407)	1.492(12)
Na(3B)-O(2B)#2	2.269(3)	C(402)-C(403)	1.596(12)
Na(3B)-O(3B)	2.292(3)	C(403)-C(404)	1.497(15)
Na(3B)-O(601)	2.324(5)	C(404)-C(405)	1.501(13)
Na(3B)-C(3B)	2.677(4)	C(405)-C(406)	1.550(12)
Na(3B)-C(31B)	3.070(4)	C(406)-C(408)	1.433(13)
Na(3B)-Na(1B)#2	3.127(2)	O(501)-C(501)	1.208(7)
Na(3B)-Na(2B)#2	3.151(2)	C(501)-C(506)	1.485(9)
O(3B)-C(31B)	1.334(4)	C(501)-C(502)	1.507(10)
O(3B)-Na(1B)#2	2.269(3)	C(502)-C(507)	1.535(11)
C(3B)-C(4B)	1.435(6)	C(502)-C(503)	1.552(11)
C(4B)-C(9B)	1.379(6)	C(503)-C(504)	1.539(12)
C(4B)-C(5B)	1.554(6)	C(504)-C(505)	1.493(11)
C(5B)-C(6B)	1.521(8)	C(505)-C(506)	1.520(9)
C(5B)-C(8B)	1.534(7)	C(506)-C(508)	1.537(10)
C(5B)-C(7B)	1.548(7)	O(601)-C(601)	1.148(9)
C(9B)-C(10B)	1.386(7)	C(601)-C(602)	1.440(13)
C(10B)-C(15B)	1.383(6)	C(601)-C(606)	1.521(13)
C(10B)-C(11B)	1.539(7)	C(602)-C(607)	1.373(14)
C(11B)-C(13C)	1.471(18)	C(602)-C(603)	1.469(14)
C(11B)-C(13D)	1.486(19)	C(603)-C(604)	1.534(16)
C(11B)-C(14D)	1.49(2)	C(604)-C(605)	1.493(17)
C(11B)-C(12C)	1.494(15)	C(605)-C(606)	1.548(16)
C(11B)-C(12D)	1.587(19)	C(606)-C(608)	1.421(14)
O(801)-O(801)#3	0.90(3)	C(901)-C(906)	1.70(4)
O(801)-C(802)#3	1.098(19)	C(902)-C(906)	1.15(3)
O(801)-C(804)#3	1.29(3)	C(902)-C(909)	1.38(3)
O(801)-C(802)	1.75(3)	O(901)-C(905)	1.161(19)
C(801)-C(802)	1.27(3)	O(901)-C(906)	1.164(19)
C(802)-O(801)#3	1.098(19)	C(904)-C(905)	1.16(3)
O(803)-C(804)	1.61(4)	C(907)-O(902)	1.162(19)

C(804)-O(801)#3	1.29(3)	C(907)-C(908)	1.39(3)
C(901)-C(902)	0.99(6)	O(902)-C(909)	1.16(2)
C(901)-C(909)	1.38(3)		

O(3)#1-Na(1)-O(101)	126.57(15)	C(3)-Na(3)-Na(1)#1	137.76(11)
O(3)#1-Na(1)-O(1)	94.93(11)	C(2)-Na(3)-Na(1)#1	127.03(10)
O(101)-Na(1)-O(1)	111.89(15)	C(31)-Na(3)-Na(1)#1	69.52(8)
O(3)#1-Na(1)-O(2)	90.71(10)	C(1)-Na(3)-Na(1)#1	97.64(9)
O(101)-Na(1)-O(2)	118.17(15)	Na(2)#1-Na(3)-Na(1)#1	82.57(5)
O(1)-Na(1)-O(2)	111.19(11)	O(2)#1-Na(3)-Na(2)	86.02(8)
O(3)#1-Na(1)-C(17)	119.51(12)	O(3)-Na(3)-Na(2)	28.92(7)
O(101)-Na(1)-C(17)	92.59(15)	O(301)-Na(3)-Na(2)	135.98(15)
O(1)-Na(1)-C(17)	112.21(12)	O(1)-Na(3)-Na(2)	87.01(8)
O(2)-Na(1)-C(17)	29.71(11)	C(3)-Na(3)-Na(2)	95.35(10)
O(3)#1-Na(1)-C(16)	139.01(12)	C(2)-Na(3)-Na(2)	78.24(9)
O(101)-Na(1)-C(16)	89.13(14)	C(31)-Na(3)-Na(2)	41.20(8)
O(1)-Na(1)-C(16)	87.86(11)	C(1)-Na(3)-Na(2)	48.83(8)
O(2)-Na(1)-C(16)	50.97(10)	Na(2)#1-Na(3)-Na(2)	89.33(5)
C(17)-Na(1)-C(16)	28.08(12)	Na(1)#1-Na(3)-Na(2)	48.82(4)
O(3)#1-Na(1)-C(3)	118.64(12)	O(2)#1-Na(3)-Na(1)	85.74(8)
O(101)-Na(1)-C(3)	95.27(15)	O(3)-Na(3)-Na(1)	89.04(8)
O(1)-Na(1)-C(3)	23.71(10)	O(301)-Na(3)-Na(1)	135.46(13)
O(2)-Na(1)-C(3)	107.94(11)	O(1)-Na(3)-Na(1)	26.81(7)
C(17)-Na(1)-C(3)	97.46(13)	C(3)-Na(3)-Na(1)	47.31(9)
C(16)-Na(1)-C(3)	70.04(11)	C(2)-Na(3)-Na(1)	55.24(8)
O(3)#1-Na(1)-Na(2)#1	49.07(8)	C(31)-Na(3)-Na(1)	90.63(8)
O(101)-Na(1)-Na(2)#1	131.15(14)	C(1)-Na(3)-Na(1)	48.84(8)
O(1)-Na(1)-Na(2)#1	46.17(8)	Na(2)#1-Na(3)-Na(1)	48.27(4)
O(2)-Na(1)-Na(2)#1	110.67(9)	Na(1)#1-Na(3)-Na(1)	91.14(5)
C(17)-Na(1)-Na(2)#1	134.28(10)	Na(2)-Na(3)-Na(1)	60.64(4)
C(16)-Na(1)-Na(2)#1	124.44(9)	C(31)-O(3)-Na(1)#1	158.5(2)
C(3)-Na(1)-Na(2)#1	69.81(9)	C(31)-O(3)-Na(3)	112.2(2)
O(3)#1-Na(1)-Na(3)#1	45.83(7)	Na(1)#1-O(3)-Na(3)	88.42(10)
O(101)-Na(1)-Na(3)#1	134.78(14)	C(31)-O(3)-Na(2)	89.0(2)
O(1)-Na(1)-Na(3)#1	113.19(9)	Na(1)#1-O(3)-Na(2)	84.27(10)
O(2)-Na(1)-Na(3)#1	45.26(7)	Na(3)-O(3)-Na(2)	123.29(12)
C(17)-Na(1)-Na(3)#1	73.69(10)	O(1)-C(3)-C(2)	120.4(4)
C(16)-Na(1)-Na(3)#1	95.81(9)	O(1)-C(3)-C(4)	121.8(4)
C(3)-Na(1)-Na(3)#1	128.65(9)	C(2)-C(3)-C(4)	117.7(4)
Na(2)#1-Na(1)-Na(3)#1	81.03(5)	O(1)-C(3)-Na(3)	62.39(19)
O(3)#1-Na(1)-Na(3)	87.45(8)	C(2)-C(3)-Na(3)	86.1(2)
O(101)-Na(1)-Na(3)	135.57(13)	C(4)-C(3)-Na(3)	120.8(3)
O(1)-Na(1)-Na(3)	27.96(7)	O(1)-C(3)-Na(1)	43.98(17)
O(2)-Na(1)-Na(3)	84.41(8)	C(2)-C(3)-Na(1)	94.2(2)
C(17)-Na(1)-Na(3)	93.03(9)	C(4)-C(3)-Na(1)	133.5(3)
C(16)-Na(1)-Na(3)	76.19(8)	Na(3)-C(3)-Na(1)	92.39(12)
C(3)-Na(1)-Na(3)	40.30(8)	C(9)-C(4)-C(3)	118.0(4)
Na(2)#1-Na(1)-Na(3)	48.42(4)	C(9)-C(4)-C(5)	120.9(4)
Na(3)#1-Na(1)-Na(3)	88.86(5)	C(3)-C(4)-C(5)	121.1(4)
O(3)#1-Na(1)-Na(2)	85.06(8)	C(6)-C(5)-C(8)	110.7(4)
O(101)-Na(1)-Na(2)	139.24(13)	C(6)-C(5)-C(4)	111.3(4)
O(1)-Na(1)-Na(2)	86.52(8)	C(8)-C(5)-C(4)	109.4(4)
O(2)-Na(1)-Na(2)	25.88(7)	C(6)-C(5)-C(7)	106.1(4)
C(17)-Na(1)-Na(2)	46.75(9)	C(8)-C(5)-C(7)	107.1(4)
C(16)-Na(1)-Na(2)	54.24(8)	C(4)-C(5)-C(7)	112.2(4)
C(3)-Na(1)-Na(2)	88.60(9)	C(10)-C(9)-C(4)	124.6(4)
Na(2)#1-Na(1)-Na(2)	88.18(5)	C(15)-C(10)-C(9)	116.6(4)
Na(3)#1-Na(1)-Na(2)	48.13(4)	C(15)-C(10)-C(11)	122.1(5)
Na(3)-Na(1)-Na(2)	59.00(4)	C(9)-C(10)-C(11)	121.3(4)
C(3)-O(1)-Na(2)#1	160.4(3)	C(13B)-C(11)-C(14A)	140.5(9)
C(3)-O(1)-Na(1)	112.3(2)	C(13B)-C(11)-C(10)	110.0(8)
Na(2)#1-O(1)-Na(1)	86.65(11)	C(14A)-C(11)-C(10)	108.7(6)
C(3)-O(1)-Na(3)	88.0(2)	C(13B)-C(11)-C(12A)	52.7(12)

Na(2)#1-O(1)-Na(3)	84.74(10)	C(14A)-C(11)-C(12A)	106.2(9)
Na(1)-O(1)-Na(3)	125.23(12)	C(10)-C(11)-C(12A)	109.9(6)
C(2)-C(1)-C(30)	112.7(3)	C(13B)-C(11)-C(12B)	110.2(17)
C(2)-C(1)-C(16)	112.5(3)	C(14A)-C(11)-C(12B)	46.5(14)
C(30)-C(1)-C(16)	112.0(3)	C(10)-C(11)-C(12B)	111.3(11)
C(2)-C(1)-Na(3)	71.1(2)	C(12A)-C(11)-C(12B)	61.5(15)
C(30)-C(1)-Na(3)	89.0(2)	C(13B)-C(11)-C(13A)	60.0(13)
C(16)-C(1)-Na(3)	153.2(3)	C(14A)-C(11)-C(13A)	111.3(9)
C(2)-C(1)-Na(2)	153.7(2)	C(10)-C(11)-C(13A)	111.7(5)
C(30)-C(1)-Na(2)	70.9(2)	C(12A)-C(11)-C(13A)	108.9(9)
C(16)-C(1)-Na(2)	88.2(2)	C(12B)-C(11)-C(13A)	136.4(12)
Na(3)-C(1)-Na(2)	83.14(10)	C(13B)-C(11)-C(14B)	109(2)
O(1)#1-Na(2)-O(201)	131.10(18)	C(14A)-C(11)-C(14B)	64.7(16)
O(1)#1-Na(2)-O(2)	95.37(11)	C(10)-C(11)-C(14B)	108.1(9)
O(201)-Na(2)-O(2)	107.2(2)	C(12A)-C(11)-C(14B)	141.8(10)
O(1)#1-Na(2)-O(3)	93.54(10)	C(12B)-C(11)-C(14B)	108(2)
O(201)-Na(2)-O(3)	114.8(2)	C(13A)-C(11)-C(14B)	51.2(16)
O(2)-Na(2)-O(3)	113.42(11)	C(10)-C(15)-C(2)	123.1(4)
O(1)#1-Na(2)-C(31)	122.09(12)	C(29)-C(16)-C(17)	119.9(4)
O(201)-Na(2)-C(31)	87.85(19)	C(29)-C(16)-C(1)	120.4(3)
O(2)-Na(2)-C(31)	113.70(12)	C(17)-C(16)-C(1)	119.7(3)
O(3)-Na(2)-C(31)	29.63(10)	C(29)-C(16)-Na(1)	127.5(3)
O(1)#1-Na(2)-C(30)	142.27(12)	C(17)-C(16)-Na(1)	63.8(2)
O(201)-Na(2)-C(30)	82.30(17)	C(1)-C(16)-Na(1)	81.1(2)
O(2)-Na(2)-C(30)	88.67(11)	O(2)-C(17)-C(16)	120.1(3)
O(3)-Na(2)-C(30)	51.25(10)	O(2)-C(17)-C(18)	121.3(4)
C(31)-Na(2)-C(30)	28.40(11)	C(16)-C(17)-C(18)	118.5(4)
O(1)#1-Na(2)-C(17)	119.30(12)	O(2)-C(17)-Na(1)	62.24(19)
O(201)-Na(2)-C(17)	88.9(2)	C(16)-C(17)-Na(1)	88.1(2)
O(2)-Na(2)-C(17)	23.95(10)	C(18)-C(17)-Na(1)	118.5(3)
O(3)-Na(2)-C(17)	109.69(11)	O(2)-C(17)-Na(2)	43.98(17)
C(31)-Na(2)-C(17)	98.43(12)	C(16)-C(17)-Na(2)	93.5(2)
C(30)-Na(2)-C(17)	70.54(11)	C(18)-C(17)-Na(2)	133.7(3)
O(1)#1-Na(2)-C(1)	127.82(11)	Na(1)-C(17)-Na(2)	93.20(12)
O(201)-Na(2)-C(1)	101.02(17)	C(23)-C(18)-C(17)	118.2(4)
O(2)-Na(2)-C(1)	61.74(10)	C(23)-C(18)-C(19)	120.6(4)
O(3)-Na(2)-C(1)	61.31(10)	C(17)-C(18)-C(19)	121.2(4)
C(31)-Na(2)-C(1)	52.00(11)	C(21)-C(19)-C(20)	110.2(4)
C(30)-Na(2)-C(1)	29.27(10)	C(21)-C(19)-C(22)	106.6(5)
C(17)-Na(2)-C(1)	49.14(11)	C(20)-C(19)-C(22)	107.5(4)
O(1)#1-Na(2)-Na(1)#1	47.18(8)	C(21)-C(19)-C(18)	110.7(4)
O(201)-Na(2)-Na(1)#1	137.6(2)	C(20)-C(19)-C(18)	109.7(4)
O(2)-Na(2)-Na(1)#1	115.25(9)	C(22)-C(19)-C(18)	112.1(4)
O(3)-Na(2)-Na(1)#1	46.66(7)	C(18)-C(23)-C(24)	123.9(4)
C(31)-Na(2)-Na(1)#1	74.95(9)	C(29)-C(24)-C(23)	116.7(4)
C(30)-Na(2)-Na(1)#1	97.51(9)	C(29)-C(24)-C(25)	123.0(4)
C(17)-Na(2)-Na(1)#1	131.32(10)	C(23)-C(24)-C(25)	120.3(4)
C(1)-Na(2)-Na(1)#1	98.18(9)	C(27)-C(25)-C(28)	108.6(5)
O(1)#1-Na(2)-Na(3)#1	49.37(8)	C(27)-C(25)-C(26)	109.7(5)
O(201)-Na(2)-Na(3)#1	130.20(19)	C(28)-C(25)-C(26)	106.4(5)
O(2)-Na(2)-Na(3)#1	46.33(7)	C(27)-C(25)-C(24)	111.3(4)
O(3)-Na(2)-Na(3)#1	114.77(9)	C(28)-C(25)-C(24)	112.0(4)
C(31)-Na(2)-Na(3)#1	138.22(11)	C(26)-C(25)-C(24)	108.7(4)
C(30)-Na(2)-Na(3)#1	127.04(10)	C(24)-C(29)-C(16)	122.7(4)
C(17)-Na(2)-Na(3)#1	70.08(8)	C(43)-C(30)-C(31)	119.1(4)
C(1)-Na(2)-Na(3)#1	97.90(9)	C(43)-C(30)-C(1)	120.5(3)
Na(1)#1-Na(2)-Na(3)#1	83.31(5)	C(31)-C(30)-C(1)	120.3(3)
O(1)#1-Na(2)-Na(3)	87.78(8)	C(43)-C(30)-Na(2)	127.8(3)
O(201)-Na(2)-Na(3)	135.01(17)	C(31)-C(30)-Na(2)	64.7(2)
O(2)-Na(2)-Na(3)	86.96(8)	C(1)-C(30)-Na(2)	79.8(2)
O(3)-Na(2)-Na(3)	27.79(7)	O(3)-C(31)-C(30)	119.5(3)
C(31)-Na(2)-Na(3)	48.14(9)	O(3)-C(31)-C(32)	122.3(3)
C(30)-Na(2)-Na(3)	54.91(8)	C(30)-C(31)-C(32)	118.2(3)

C(17)-Na(2)-Na(3)	89.12(9)	O(3)-C(31)-Na(2)	61.41(19)
C(1)-Na(2)-Na(3)	48.03(8)	C(30)-C(31)-Na(2)	86.9(2)
Na(1)#1-Na(2)-Na(3)	50.16(4)	C(32)-C(31)-Na(2)	120.2(3)
Na(3)#1-Na(2)-Na(3)	90.67(5)	O(3)-C(31)-Na(3)	43.88(17)
O(1)#1-Na(2)-Na(1)	88.98(8)	C(30)-C(31)-Na(3)	92.0(2)
O(201)-Na(2)-Na(1)	128.8(2)	C(32)-C(31)-Na(3)	135.9(3)
O(2)-Na(2)-Na(1)	27.10(7)	Na(2)-C(31)-Na(3)	90.66(12)
O(3)-Na(2)-Na(1)	87.64(8)	C(37)-C(32)-C(31)	118.8(4)
C(31)-Na(2)-Na(1)	95.64(10)	C(37)-C(32)-C(33)	119.8(4)
C(30)-Na(2)-Na(1)	77.83(8)	C(31)-C(32)-C(33)	121.3(4)
C(17)-Na(2)-Na(1)	40.04(8)	C(34)-C(33)-C(36)	107.8(4)
C(1)-Na(2)-Na(1)	48.61(8)	C(34)-C(33)-C(35)	106.9(4)
Na(1)#1-Na(2)-Na(1)	91.82(5)	C(36)-C(33)-C(35)	109.5(4)
Na(3)#1-Na(2)-Na(1)	49.29(4)	C(34)-C(33)-C(32)	112.3(4)
Na(3)-Na(2)-Na(1)	60.36(4)	C(36)-C(33)-C(32)	111.3(4)
C(17)-O(2)-Na(3)#1	159.2(3)	C(35)-C(33)-C(32)	108.9(4)
C(17)-O(2)-Na(2)	112.1(2)	C(32)-C(37)-C(38)	123.7(4)
Na(3)#1-O(2)-Na(2)	87.04(10)	C(43)-C(38)-C(37)	116.3(4)
C(17)-O(2)-Na(1)	88.0(2)	C(43)-C(38)-C(39)	123.4(4)
Na(3)#1-O(2)-Na(1)	86.58(10)	C(37)-C(38)-C(39)	120.3(4)
Na(2)-O(2)-Na(1)	127.03(12)	C(41)-C(39)-C(38)	112.1(4)
C(15)-C(2)-C(3)	119.9(4)	C(41)-C(39)-C(40)	107.9(4)
C(15)-C(2)-C(1)	120.6(4)	C(38)-C(39)-C(40)	110.4(5)
C(3)-C(2)-C(1)	119.5(3)	C(41)-C(39)-C(42)	107.9(5)
C(15)-C(2)-Na(3)	128.5(3)	C(38)-C(39)-C(42)	108.6(4)
C(3)-C(2)-Na(3)	65.3(2)	C(40)-C(39)-C(42)	110.0(5)
C(1)-C(2)-Na(3)	79.4(2)	C(38)-C(43)-C(30)	123.8(4)
O(2)#1-Na(3)-O(3)	93.51(11)	C(101)-O(101)-Na(1)	176.4(4)
O(2)#1-Na(3)-O(301)	128.73(15)	O(101)-C(101)-C(106)	125.3(6)
O(3)-Na(3)-O(301)	112.19(17)	O(101)-C(101)-C(102)	120.1(5)
O(2)#1-Na(3)-O(1)	92.20(11)	C(106)-C(101)-C(102)	114.6(5)
O(3)-Na(3)-O(1)	114.59(11)	C(103)-C(102)-C(101)	112.2(7)
O(301)-Na(3)-O(1)	113.54(15)	C(103)-C(102)-C(107)	115.1(9)
O(2)#1-Na(3)-C(3)	121.03(13)	C(101)-C(102)-C(107)	107.4(8)
O(3)-Na(3)-C(3)	114.79(12)	C(102)-C(103)-C(104)	107.7(10)
O(301)-Na(3)-C(3)	88.25(15)	C(105)-C(104)-C(103)	106.9(8)
O(1)-Na(3)-C(3)	29.58(11)	C(106)-C(105)-C(104)	113.0(9)
O(2)#1-Na(3)-C(2)	140.81(12)	C(105)-C(106)-C(101)	110.1(7)
O(3)-Na(3)-C(2)	89.70(11)	C(105)-C(106)-C(108)	112.9(7)
O(301)-Na(3)-C(2)	85.02(14)	C(101)-C(106)-C(108)	114.3(6)
O(1)-Na(3)-C(2)	51.73(10)	C(201)-O(201)-Na(2)	172.0(7)
C(3)-Na(3)-C(2)	28.62(12)	O(201)-C(201)-C(206)	145.3(12)
O(2)#1-Na(3)-C(31)	117.39(11)	O(201)-C(201)-C(202)	109.3(10)
O(3)-Na(3)-C(31)	23.88(10)	C(206)-C(201)-C(202)	105.3(12)
O(301)-Na(3)-C(31)	94.88(16)	C(203)-C(202)-C(207)	112.9(16)
O(1)-Na(3)-C(31)	110.54(11)	C(203)-C(202)-C(201)	117.6(14)
C(3)-Na(3)-C(31)	99.26(12)	C(207)-C(202)-C(201)	111.2(14)
C(2)-Na(3)-C(31)	71.24(11)	C(204)-C(203)-C(202)	102.3(13)
O(2)#1-Na(3)-C(1)	125.54(11)	C(203)-C(204)-C(205)	125.9(15)
O(3)-Na(3)-C(1)	62.67(10)	C(206)-C(205)-C(204)	100.7(14)
O(301)-Na(3)-C(1)	105.73(14)	C(205)-C(206)-C(201)	121.1(19)
O(1)-Na(3)-C(1)	61.69(10)	C(205)-C(206)-C(208)	106.9(11)
C(3)-Na(3)-C(1)	52.15(12)	C(201)-C(206)-C(208)	109.5(11)
C(2)-Na(3)-C(1)	29.51(11)	C(301)-O(301)-Na(3)	158.7(5)
C(31)-Na(3)-C(1)	49.68(10)	O(301)-C(301)-C(302)	131.1(8)
O(2)#1-Na(3)-Na(2)#1	46.63(8)	O(301)-C(301)-C(306)	112.8(7)
O(3)-Na(3)-Na(2)#1	114.43(9)	C(302)-C(301)-C(306)	116.1(9)
O(301)-Na(3)-Na(2)#1	133.34(16)	C(301)-C(302)-C(307)	117.4(9)
O(1)-Na(3)-Na(2)#1	45.89(7)	C(301)-C(302)-C(303)	109.3(8)
C(3)-Na(3)-Na(2)#1	74.41(10)	C(307)-C(302)-C(303)	111.3(11)
C(2)-Na(3)-Na(2)#1	97.05(9)	C(304)-C(303)-C(302)	100.1(10)
C(31)-Na(3)-Na(2)#1	130.07(9)	C(305)-C(304)-C(303)	113.4(10)
C(1)-Na(3)-Na(2)#1	97.09(9)	C(304)-C(305)-C(306)	106.8(10)

O(2)#1-Na(3)-Na(1)#1	48.16(8)	C(308)-C(306)-C(301)	117.7(10)
O(3)-Na(3)-Na(1)#1	45.74(7)	C(308)-C(306)-C(305)	114.2(11)
O(301)-Na(3)-Na(1)#1	132.03(14)	C(301)-C(306)-C(305)	105.9(9)
O(1)-Na(3)-Na(1)#1	114.42(9)		
O(3B)#2-Na(1B)-O(401)	127.23(15)	O(2B)#2-Na(3B)-Na(1B)	85.75(8)
O(3B)#2-Na(1B)-O(1B)	94.71(11)	O(3B)-Na(3B)-Na(1B)	87.02(8)
O(401)-Na(1B)-O(1B)	113.99(17)	O(601)-Na(3B)-Na(1B)	137.31(15)
O(3B)#2-Na(1B)-O(2B)	92.89(11)	O(1B)-Na(3B)-Na(1B)	27.06(7)
O(401)-Na(1B)-O(2B)	112.39(14)	C(3B)-Na(3B)-Na(1B)	48.04(9)
O(1B)-Na(1B)-O(2B)	113.38(11)	C(2B)-Na(3B)-Na(1B)	55.28(8)
O(3B)#2-Na(1B)-C(17B)	121.83(12)	C(31B)-Na(3B)-Na(1B)	88.78(8)
O(401)-Na(1B)-C(17B)	86.84(14)	Na(1B)#2-Na(3B)-Na(1B)	89.58(5)
O(1B)-Na(1B)-C(17B)	113.87(12)	Na(2B)#2-Na(3B)-Na(1B)	48.80(4)
O(2B)-Na(1B)-C(17B)	29.95(10)	O(2B)#2-Na(3B)-Na(2B)	87.59(8)
O(3B)#2-Na(1B)-C(16B)	141.97(12)	O(3B)-Na(3B)-Na(2B)	27.84(7)
O(401)-Na(1B)-C(16B)	84.54(13)	O(601)-Na(3B)-Na(2B)	132.55(18)
O(1B)-Na(1B)-C(16B)	88.66(11)	O(1B)-Na(3B)-Na(2B)	86.26(8)
O(2B)-Na(1B)-C(16B)	51.82(10)	C(3B)-Na(3B)-Na(2B)	94.96(10)
C(17B)-Na(1B)-C(16B)	28.69(12)	C(2B)-Na(3B)-Na(2B)	77.49(8)
O(3B)#2-Na(1B)-C(3B)	118.02(11)	C(31B)-Na(3B)-Na(2B)	40.16(8)
O(401)-Na(1B)-C(3B)	96.94(17)	Na(1B)#2-Na(3B)-Na(2B)	48.79(4)
O(1B)-Na(1B)-C(3B)	23.31(10)	Na(2B)#2-Na(3B)-Na(2B)	90.01(5)
O(2B)-Na(1B)-C(3B)	109.29(11)	Na(1B)-Na(3B)-Na(2B)	59.71(4)
C(17B)-Na(1B)-C(3B)	98.52(12)	C(31B)-O(3B)-Na(1B)#2	159.5(2)
C(16B)-Na(1B)-C(3B)	70.48(11)	C(31B)-O(3B)-Na(3B)	113.0(2)
O(3B)#2-Na(1B)-C(1B)	127.08(11)	Na(1B)#2-O(3B)-Na(3B)	86.59(10)
O(401)-Na(1B)-C(1B)	105.63(14)	C(31B)-O(3B)-Na(2B)	87.6(2)
O(1B)-Na(1B)-C(1B)	62.01(10)	Na(1B)#2-O(3B)-Na(2B)	85.22(10)
O(2B)-Na(1B)-C(1B)	61.30(10)	Na(3B)-O(3B)-Na(2B)	125.44(13)
C(17B)-Na(1B)-C(1B)	51.89(11)	O(1B)-C(3B)-C(2B)	120.1(3)
C(16B)-Na(1B)-C(1B)	29.08(10)	O(1B)-C(3B)-C(4B)	122.1(4)
C(3B)-Na(1B)-C(1B)	49.01(10)	C(2B)-C(3B)-C(4B)	117.7(4)
O(3B)#2-Na(1B)-Na(3B)#2	47.02(8)	O(1B)-C(3B)-Na(3B)	62.98(19)
O(401)-Na(1B)-Na(3B)#2	130.97(16)	C(2B)-C(3B)-Na(3B)	87.7(2)
O(1B)-Na(1B)-Na(3B)#2	115.02(9)	C(4B)-C(3B)-Na(3B)	117.8(3)
O(2B)-Na(1B)-Na(3B)#2	46.24(7)	O(1B)-C(3B)-Na(1B)	42.84(17)
C(17B)-Na(1B)-Na(3B)#2	74.83(9)	C(2B)-C(3B)-Na(1B)	92.9(2)
C(16B)-Na(1B)-Na(3B)#2	97.66(9)	C(4B)-C(3B)-Na(1B)	136.5(3)
C(3B)-Na(1B)-Na(3B)#2	130.14(9)	Na(3B)-C(3B)-Na(1B)	91.76(12)
C(1B)-Na(1B)-Na(3B)#2	97.93(9)	C(9B)-C(4B)-C(3B)	118.7(4)
O(3B)#2-Na(1B)-Na(2B)#2	48.88(8)	C(9B)-C(4B)-C(5B)	120.7(4)
O(401)-Na(1B)-Na(2B)#2	133.75(13)	C(3B)-C(4B)-C(5B)	120.6(4)
O(1B)-Na(1B)-Na(2B)#2	46.14(7)	C(6B)-C(5B)-C(8B)	110.5(4)
O(2B)-Na(1B)-Na(2B)#2	113.83(9)	C(6B)-C(5B)-C(7B)	106.7(5)
C(17B)-Na(1B)-Na(2B)#2	137.60(10)	C(8B)-C(5B)-C(7B)	106.5(5)
C(16B)-Na(1B)-Na(2B)#2	126.57(9)	C(6B)-C(5B)-C(4B)	111.3(4)
C(3B)-Na(1B)-Na(2B)#2	69.35(8)	C(8B)-C(5B)-C(4B)	109.6(4)
C(1B)-Na(1B)-Na(2B)#2	97.60(9)	C(7B)-C(5B)-C(4B)	112.2(4)
Na(3B)#2-Na(1B)-Na(2B)#2	82.85(5)	C(4B)-C(9B)-C(10B)	124.3(4)
O(3B)#2-Na(1B)-Na(2B)	86.71(8)	C(15B)-C(10B)-C(9B)	116.5(4)
O(401)-Na(1B)-Na(2B)	134.68(12)	C(15B)-C(10B)-C(11B)	121.9(5)
O(1B)-Na(1B)-Na(2B)	87.96(8)	C(9B)-C(10B)-C(11B)	121.6(4)
O(2B)-Na(1B)-Na(2B)	26.79(7)	C(13C)-C(11B)-C(13D)	39.4(8)
C(17B)-Na(1B)-Na(2B)	47.88(8)	C(13C)-C(11B)-C(14D)	132.3(11)
C(16B)-Na(1B)-Na(2B)	55.52(8)	C(13D)-C(11B)-C(14D)	111.9(13)
C(3B)-Na(1B)-Na(2B)	89.43(8)	C(13C)-C(11B)-C(12C)	117.0(12)
C(1B)-Na(1B)-Na(2B)	48.83(8)	C(13D)-C(11B)-C(12C)	139.5(10)
Na(3B)#2-Na(1B)-Na(2B)	49.10(4)	C(14D)-C(11B)-C(12C)	54.1(12)
Na(2B)#2-Na(1B)-Na(2B)	90.43(5)	C(13C)-C(11B)-C(10B)	113.6(7)
O(3B)#2-Na(1B)-Na(3B)	87.57(8)	C(13D)-C(11B)-C(10B)	112.1(9)
O(401)-Na(1B)-Na(3B)	136.98(15)	C(14D)-C(11B)-C(10B)	113.1(10)
O(1B)-Na(1B)-Na(3B)	28.28(7)	C(12C)-C(11B)-C(10B)	108.0(7)

O(2B)-Na(1B)-Na(3B)	86.50(8)	C(13C)-C(11B)-C(12D)	66.8(11)
C(17B)-Na(1B)-Na(3B)	95.15(9)	C(13D)-C(11B)-C(12D)	104.5(12)
C(16B)-Na(1B)-Na(3B)	77.74(8)	C(14D)-C(11B)-C(12D)	105.9(13)
C(3B)-Na(1B)-Na(3B)	40.20(8)	C(12C)-C(11B)-C(12D)	56.1(10)
C(1B)-Na(1B)-Na(3B)	48.74(8)	C(10B)-C(11B)-C(12D)	108.7(7)
Na(3B)#2-Na(1B)-Na(3B)	90.42(5)	C(13C)-C(11B)-C(14C)	110.3(10)
Na(2B)#2-Na(1B)-Na(3B)	48.86(4)	C(13D)-C(11B)-C(14C)	73.7(11)
Na(2B)-Na(1B)-Na(3B)	60.21(4)	C(14D)-C(11B)-C(14C)	46.3(10)
C(3B)-O(1B)-Na(2B)#2	158.2(3)	C(12C)-C(11B)-C(14C)	100.2(11)
C(3B)-O(1B)-Na(1B)	113.9(2)	C(10B)-C(11B)-C(14C)	106.5(6)
Na(2B)#2-O(1B)-Na(1B)	87.18(10)	C(12D)-C(11B)-C(14C)	142.3(8)
C(3B)-O(1B)-Na(3B)	87.2(2)	C(10B)-C(15B)-C(2B)	123.2(4)
Na(2B)#2-O(1B)-Na(3B)	85.04(10)	C(29B)-C(16B)-C(17B)	119.7(3)
Na(1B)-O(1B)-Na(3B)	124.66(12)	C(29B)-C(16B)-C(1B)	120.3(4)
C(16B)-C(1B)-C(2B)	113.5(3)	C(17B)-C(16B)-C(1B)	120.0(3)
C(16B)-C(1B)-C(30B)	112.8(3)	C(29B)-C(16B)-Na(1B)	128.6(3)
C(2B)-C(1B)-C(30B)	112.3(3)	C(17B)-C(16B)-Na(1B)	64.4(2)
C(16B)-C(1B)-Na(1B)	70.25(19)	C(1B)-C(16B)-Na(1B)	80.7(2)
C(2B)-C(1B)-Na(1B)	89.8(2)	O(2B)-C(17B)-C(16B)	120.0(3)
C(30B)-C(1B)-Na(1B)	151.9(3)	O(2B)-C(17B)-C(18B)	121.6(4)
O(1B)#2-Na(2B)-O(2B)	94.69(11)	C(16B)-C(17B)-C(18B)	118.4(3)
O(1B)#2-Na(2B)-O(501)	124.85(16)	O(2B)-C(17B)-Na(1B)	62.49(18)
O(2B)-Na(2B)-O(501)	114.98(17)	C(16B)-C(17B)-Na(1B)	86.9(2)
O(1B)#2-Na(2B)-O(3B)	92.29(10)	C(18B)-C(17B)-Na(1B)	120.1(3)
O(2B)-Na(2B)-O(3B)	112.94(11)	O(2B)-C(17B)-Na(2B)	42.99(17)
O(501)-Na(2B)-O(3B)	114.13(16)	C(16B)-C(17B)-Na(2B)	93.7(2)
O(1B)#2-Na(2B)-C(31B)	121.21(12)	C(18B)-C(17B)-Na(2B)	133.9(3)
O(2B)-Na(2B)-C(31B)	113.36(12)	Na(1B)-C(17B)-Na(2B)	91.78(11)
O(501)-Na(2B)-C(31B)	89.41(15)	C(23B)-C(18B)-C(17B)	118.1(4)
O(3B)-Na(2B)-C(31B)	29.83(10)	C(23B)-C(18B)-C(19B)	120.6(4)
O(1B)#2-Na(2B)-C(30B)	140.99(12)	C(17B)-C(18B)-C(19B)	121.3(4)
O(2B)-Na(2B)-C(30B)	88.49(11)	C(21B)-C(19B)-C(18B)	111.2(4)
O(501)-Na(2B)-C(30B)	87.76(15)	C(21B)-C(19B)-C(20B)	111.2(4)
O(3B)-Na(2B)-C(30B)	51.49(10)	C(18B)-C(19B)-C(20B)	109.6(4)
C(31B)-Na(2B)-C(30B)	28.38(11)	C(21B)-C(19B)-C(22B)	106.7(4)
O(1B)#2-Na(2B)-C(17B)	118.28(11)	C(18B)-C(19B)-C(22B)	111.9(4)
O(2B)-Na(2B)-C(17B)	23.59(10)	C(20B)-C(19B)-C(22B)	106.0(4)
O(501)-Na(2B)-C(17B)	98.34(16)	C(18B)-C(23B)-C(24B)	124.5(4)
O(3B)-Na(2B)-C(17B)	109.05(11)	C(23B)-C(24B)-C(29B)	116.7(4)
C(31B)-Na(2B)-C(17B)	98.09(12)	C(23B)-C(24B)-C(25B)	120.0(4)
C(30B)-Na(2B)-C(17B)	70.33(11)	C(29B)-C(24B)-C(25B)	123.2(4)
O(1B)#2-Na(2B)-Na(1B)#2	46.68(8)	C(26B)-C(25B)-C(28B)	109.6(6)
O(2B)-Na(2B)-Na(1B)#2	114.05(9)	C(26B)-C(25B)-C(24B)	111.3(4)
O(501)-Na(2B)-Na(1B)#2	130.84(16)	C(28B)-C(25B)-C(24B)	107.9(4)
O(3B)-Na(2B)-Na(1B)#2	45.90(7)	C(26B)-C(25B)-C(27B)	108.2(5)
C(31B)-Na(2B)-Na(1B)#2	74.55(9)	C(28B)-C(25B)-C(27B)	107.6(6)
C(30B)-Na(2B)-Na(1B)#2	96.89(9)	C(24B)-C(25B)-C(27B)	112.2(4)
C(17B)-Na(2B)-Na(1B)#2	129.37(9)	C(16B)-C(29B)-C(24B)	122.6(4)
O(1B)#2-Na(2B)-Na(3B)#2	49.03(8)	C(43B)-C(30B)-C(31B)	120.0(4)
O(2B)-Na(2B)-Na(3B)#2	46.01(8)	C(43B)-C(30B)-C(1B)	119.7(3)
O(501)-Na(2B)-Na(3B)#2	132.33(14)	C(31B)-C(30B)-C(1B)	120.3(3)
O(3B)-Na(2B)-Na(3B)#2	113.38(9)	C(43B)-C(30B)-Na(2B)	127.4(3)
C(31B)-Na(2B)-Na(3B)#2	136.87(10)	C(31B)-C(30B)-Na(2B)	64.3(2)
C(30B)-Na(2B)-Na(3B)#2	126.05(10)	C(1B)-C(30B)-Na(2B)	81.2(2)
C(17B)-Na(2B)-Na(3B)#2	69.50(8)	O(3B)-C(31B)-C(30B)	120.4(3)
Na(1B)#2-Na(2B)-Na(3B)#2	82.33(5)	O(3B)-C(31B)-C(32B)	121.4(3)
O(1B)#2-Na(2B)-Na(1B)	87.34(8)	C(30B)-C(31B)-C(32B)	118.2(3)
O(2B)-Na(2B)-Na(1B)	28.03(7)	O(3B)-C(31B)-Na(2B)	62.53(19)
O(501)-Na(2B)-Na(1B)	138.66(15)	C(30B)-C(31B)-Na(2B)	87.3(2)
O(3B)-Na(2B)-Na(1B)	86.29(8)	C(32B)-C(31B)-Na(2B)	118.7(3)
C(31B)-Na(2B)-Na(1B)	94.72(9)	O(3B)-C(31B)-Na(3B)	43.39(17)
C(30B)-Na(2B)-Na(1B)	77.50(8)	C(30B)-C(31B)-Na(3B)	93.7(2)
C(17B)-Na(2B)-Na(1B)	40.34(7)	C(32B)-C(31B)-Na(3B)	134.8(3)

Na(1B)#2-Na(2B)-Na(1B)	89.57(5)	Na(2B)-C(31B)-Na(3B)	92.21(11)
Na(3B)#2-Na(2B)-Na(1B)	48.60(4)	C(37B)-C(32B)-C(31B)	118.3(4)
O(1B)#2-Na(2B)-Na(3B)	86.06(8)	C(37B)-C(32B)-C(33B)	120.7(4)
O(2B)-Na(2B)-Na(3B)	87.58(8)	C(31B)-C(32B)-C(33B)	121.0(4)
O(501)-Na(2B)-Na(3B)	137.04(14)	C(35B)-C(33B)-C(34B)	109.9(4)
O(3B)-Na(2B)-Na(3B)	26.72(7)	C(35B)-C(33B)-C(32B)	111.3(4)
C(31B)-Na(2B)-Na(3B)	47.63(8)	C(34B)-C(33B)-C(32B)	109.5(4)
C(30B)-Na(2B)-Na(3B)	55.19(8)	C(35B)-C(33B)-C(36B)	107.3(4)
C(17B)-Na(2B)-Na(3B)	89.33(8)	C(34B)-C(33B)-C(36B)	106.8(5)
Na(1B)#2-Na(2B)-Na(3B)	48.36(4)	C(32B)-C(33B)-C(36B)	111.9(4)
Na(3B)#2-Na(2B)-Na(3B)	89.99(5)	C(38B)-C(37B)-C(32B)	124.2(4)
Na(1B)-Na(2B)-Na(3B)	60.07(4)	C(43B)-C(38B)-C(37B)	116.8(4)
C(17B)-O(2B)-Na(3B)#2	158.0(2)	C(43B)-C(38B)-C(39B)	122.3(4)
C(17B)-O(2B)-Na(2B)	113.4(2)	C(37B)-C(38B)-C(39B)	120.8(4)
Na(3B)#2-O(2B)-Na(2B)	87.74(10)	C(41B)-C(39B)-C(40B)	109.7(5)
C(17B)-O(2B)-Na(1B)	87.6(2)	C(41B)-C(39B)-C(38B)	109.4(4)
Na(3B)#2-O(2B)-Na(1B)	84.63(10)	C(40B)-C(39B)-C(38B)	112.3(4)
Na(2B)-O(2B)-Na(1B)	125.18(12)	C(41B)-C(39B)-C(42B)	107.6(4)
C(15B)-C(2B)-C(3B)	119.6(4)	C(40B)-C(39B)-C(42B)	107.4(4)
C(15B)-C(2B)-C(1B)	120.8(4)	C(38B)-C(39B)-C(42B)	110.3(4)
C(3B)-C(2B)-C(1B)	119.6(3)	C(38B)-C(43B)-C(30B)	122.5(4)
C(15B)-C(2B)-Na(3B)	127.6(3)	C(401)-O(401)-Na(1B)	152.5(5)
C(3B)-C(2B)-Na(3B)	63.7(2)	O(401)-C(401)-C(402)	127.7(7)
C(1B)-C(2B)-Na(3B)	81.1(2)	O(401)-C(401)-C(406)	116.0(6)
O(2B)#2-Na(3B)-O(3B)	95.14(11)	C(402)-C(401)-C(406)	116.3(7)
O(2B)#2-Na(3B)-O(601)	129.29(16)	C(401)-C(402)-C(407)	115.3(7)
O(3B)-Na(3B)-O(601)	109.41(18)	C(401)-C(402)-C(403)	105.6(7)
O(2B)#2-Na(3B)-O(1B)	91.85(11)	C(407)-C(402)-C(403)	112.3(9)
O(3B)-Na(3B)-O(1B)	112.71(11)	C(404)-C(403)-C(402)	104.3(9)
O(601)-Na(3B)-O(1B)	116.20(15)	C(403)-C(404)-C(405)	112.8(8)
O(2B)#2-Na(3B)-C(3B)	120.70(13)	C(404)-C(405)-C(406)	109.7(9)
O(3B)-Na(3B)-C(3B)	113.41(12)	C(408)-C(406)-C(401)	116.4(9)
O(601)-Na(3B)-C(3B)	89.69(15)	C(408)-C(406)-C(405)	115.6(9)
O(1B)-Na(3B)-C(3B)	29.86(11)	C(401)-C(406)-C(405)	104.9(8)
O(2B)#2-Na(3B)-C(2B)	140.70(12)	C(501)-O(501)-Na(2B)	173.1(5)
O(3B)-Na(3B)-C(2B)	88.32(11)	O(501)-C(501)-C(506)	122.3(7)
O(601)-Na(3B)-C(2B)	85.22(15)	O(501)-C(501)-C(502)	121.9(6)
O(1B)-Na(3B)-C(2B)	51.51(10)	C(506)-C(501)-C(502)	115.5(6)
C(3B)-Na(3B)-C(2B)	28.59(11)	C(501)-C(502)-C(507)	111.9(6)
O(2B)#2-Na(3B)-C(31B)	118.71(11)	C(501)-C(502)-C(503)	109.5(6)
O(3B)-Na(3B)-C(31B)	23.57(10)	C(507)-C(502)-C(503)	112.6(7)
O(601)-Na(3B)-C(31B)	92.41(18)	C(504)-C(503)-C(502)	111.8(7)
O(1B)-Na(3B)-C(31B)	108.78(11)	C(505)-C(504)-C(503)	109.8(7)
C(3B)-Na(3B)-C(31B)	98.10(12)	C(504)-C(505)-C(506)	112.9(7)
C(2B)-Na(3B)-C(31B)	70.13(11)	C(501)-C(506)-C(505)	110.1(6)
O(2B)#2-Na(3B)-Na(1B)#2	49.13(8)	C(501)-C(506)-C(508)	112.5(6)
O(3B)-Na(3B)-Na(1B)#2	46.40(8)	C(505)-C(506)-C(508)	114.0(7)
O(601)-Na(3B)-Na(1B)#2	130.59(15)	C(601)-O(601)-Na(3B)	164.4(7)
O(1B)-Na(3B)-Na(1B)#2	113.17(9)	O(601)-C(601)-C(602)	133.0(10)
C(3B)-Na(3B)-Na(1B)#2	137.00(11)	O(601)-C(601)-C(606)	108.0(9)
C(2B)-Na(3B)-Na(1B)#2	126.20(10)	C(602)-C(601)-C(606)	118.4(9)
C(31B)-Na(3B)-Na(1B)#2	69.87(8)	C(607)-C(602)-C(601)	118.4(14)
O(2B)#2-Na(3B)-Na(2B)#2	46.25(8)	C(607)-C(602)-C(603)	110.9(14)
O(3B)-Na(3B)-Na(2B)#2	114.36(9)	C(601)-C(602)-C(603)	121.3(12)
O(601)-Na(3B)-Na(2B)#2	136.21(18)	C(602)-C(603)-C(604)	107.4(11)
O(1B)-Na(3B)-Na(2B)#2	45.93(7)	C(605)-C(604)-C(603)	111.3(15)
C(3B)-Na(3B)-Na(2B)#2	74.47(10)	C(604)-C(605)-C(606)	112.8(14)
C(2B)-Na(3B)-Na(2B)#2	97.01(9)	C(608)-C(606)-C(601)	115.0(12)
C(31B)-Na(3B)-Na(2B)#2	129.59(9)	C(608)-C(606)-C(605)	109.7(16)
Na(1B)#2-Na(3B)-Na(2B)#2	82.30(6)	C(601)-C(606)-C(605)	108.9(10)
O(801)#3-O(801)-C(802)#3	122(3)	C(901)-C(902)-C(906)	105(3)
O(801)#3-O(801)-C(804)#3	79(2)	C(901)-C(902)-C(909)	69.2(15)

C(802)#3-O(801)-C(804)#3	47.8(14)	C(906)-C(902)-C(909)	36(2)
O(801)#3-O(801)-C(802)	32.2(18)	C(905)-O(901)-C(906)	153(5)
C(802)#3-O(801)-C(802)	154.1(14)	O(901)-C(905)-C(904)	137(5)
C(804)#3-O(801)-C(802)	109.0(13)	C(902)-C(906)-O(901)	137(4)
O(801)#3-C(802)-C(801)	139(2)	C(902)-C(906)-C(901)	34(2)
O(801)#3-C(802)-O(801)	25.9(14)	O(901)-C(906)-C(901)	103(4)
C(801)-C(802)-O(801)	116(2)	O(902)-C(907)-C(908)	128(4)
O(801)#3-C(804)-O(803)	101(2)	C(909)-O(902)-C(907)	134(5)
C(902)-C(901)-C(909)	69.0(14)	O(902)-C(909)-C(902)	161(5)
C(902)-C(901)-C(906)	40.8(16)	O(902)-C(909)-C(901)	126(5)
C(909)-C(901)-C(906)	28.2(16)	C(902)-C(909)-C(901)	42(3)

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

Table 47. Anisotropic displacement parameters (A^2 x 10^3) for **3a·5.6$C_8H_{14}O$** (2,6-dimethyl cyclohexanone).
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Na(1)	34(1)	31(1)	33(1)	3(1)	2(1)	5(1)
O(1)	36(2)	25(1)	30(2)	1(1)	1(1)	2(1)
C(1)	28(2)	25(2)	27(2)	6(2)	4(2)	8(2)
Na(2)	34(1)	37(1)	32(1)	1(1)	3(1)	2(1)
O(2)	28(1)	29(1)	31(2)	6(1)	0(1)	3(1)
C(2)	31(2)	27(2)	34(2)	6(2)	9(2)	8(2)
Na(3)	34(1)	30(1)	32(1)	2(1)	3(1)	3(1)
O(3)	34(2)	27(1)	24(1)	2(1)	0(1)	6(1)
C(3)	33(2)	24(2)	36(2)	2(2)	11(2)	6(2)
C(4)	40(2)	29(2)	46(3)	-7(2)	12(2)	1(2)
C(5)	56(3)	35(2)	45(3)	-8(2)	5(2)	-7(2)
C(6)	73(4)	57(3)	47(3)	-12(2)	6(3)	-13(3)
C(7)	86(4)	44(3)	78(4)	-17(3)	2(3)	-23(3)
C(8)	55(3)	52(3)	60(3)	-4(3)	-7(3)	-7(2)
C(9)	49(3)	23(2)	62(3)	0(2)	16(2)	1(2)
C(10)	48(3)	30(2)	59(3)	14(2)	13(2)	9(2)
C(11)	71(4)	31(3)	83(4)	27(3)	19(3)	9(2)
C(12A)	88(8)	79(8)	174(14)	72(9)	45(9)	13(6)
C(12B)	240(40)	25(10)	78(16)	22(10)	50(20)	-1(17)
C(13A)	166(14)	73(7)	93(9)	56(6)	-14(9)	28(8)
C(13B)	95(18)	56(13)	75(15)	53(12)	31(13)	24(12)
C(14A)	131(11)	51(6)	128(11)	44(7)	47(10)	49(7)
C(14B)	73(16)	110(20)	210(40)	120(30)	30(20)	40(16)
C(15)	41(2)	31(2)	41(2)	9(2)	7(2)	11(2)
C(16)	29(2)	32(2)	25(2)	1(2)	6(2)	6(2)
C(17)	29(2)	38(2)	24(2)	-2(2)	3(2)	7(2)
C(18)	29(2)	45(3)	32(2)	1(2)	4(2)	1(2)
C(19)	30(2)	62(3)	50(3)	13(2)	6(2)	-6(2)
C(20)	43(3)	80(4)	46(3)	22(3)	13(2)	7(3)
C(21)	56(3)	52(3)	78(4)	6(3)	-5(3)	-16(3)
C(22)	33(3)	98(5)	95(5)	38(4)	11(3)	-2(3)
C(23)	25(2)	57(3)	36(2)	-2(2)	3(2)	9(2)
C(24)	37(2)	43(2)	29(2)	-1(2)	1(2)	14(2)
C(25)	40(3)	53(3)	42(3)	2(2)	-1(2)	24(2)
C(26)	104(5)	75(4)	67(4)	-5(3)	-39(4)	44(4)

C(27)	76(4)	91(5)	61(4)	5(3)	11(3)	52(4)
C(28)	67(4)	73(4)	109(6)	36(4)	-6(4)	31(3)
C(29)	32(2)	38(2)	31(2)	2(2)	5(2)	11(2)
C(30)	27(2)	33(2)	26(2)	4(2)	3(2)	2(2)
C(31)	27(2)	29(2)	28(2)	2(2)	3(2)	1(2)
C(32)	31(2)	38(2)	28(2)	1(2)	3(2)	3(2)
C(33)	48(3)	52(3)	30(2)	-4(2)	6(2)	18(2)
C(34)	78(4)	94(4)	36(3)	-11(3)	4(3)	45(3)
C(35)	79(4)	41(3)	49(3)	-13(2)	0(3)	16(3)
C(36)	40(3)	73(4)	51(3)	8(3)	12(2)	20(2)
C(37)	37(2)	49(3)	25(2)	0(2)	2(2)	4(2)
C(38)	35(2)	48(3)	30(2)	6(2)	-3(2)	4(2)
C(39)	42(3)	80(4)	32(2)	10(2)	-7(2)	12(3)
C(40)	73(4)	99(5)	47(3)	-6(3)	-26(3)	21(3)
C(41)	45(3)	94(4)	43(3)	15(3)	-7(2)	20(3)
C(42)	70(4)	112(5)	52(3)	42(4)	4(3)	21(4)
C(43)	29(2)	42(2)	34(2)	4(2)	2(2)	8(2)
O(101)	73(3)	81(3)	76(3)	0(2)	4(2)	45(2)
C(101)	56(3)	59(3)	77(4)	13(3)	9(3)	22(3)
C(102)	94(5)	81(5)	146(8)	48(5)	48(5)	41(4)
C(103)	231(13)	110(8)	196(12)	-39(8)	163(11)	-22(8)
C(107)	64(5)	256(15)	189(12)	81(11)	6(6)	-2(7)
O(201)	158(5)	115(4)	92(4)	12(3)	-77(4)	-30(4)
C(201)	86(5)	121(7)	103(6)	23(5)	-12(5)	-3(5)
C(203)	200(14)	131(10)	193(14)	-42(9)	7(11)	-15(10)
C(206)	69(6)	570(30)	96(8)	-37(13)	-21(6)	-18(12)
C(207)	181(13)	360(20)	133(11)	9(14)	15(10)	49(15)
C(208)	233(13)	107(7)	88(6)	-21(5)	39(7)	37(7)
O(301)	67(3)	79(3)	117(4)	51(3)	31(3)	3(2)
C(301)	70(4)	47(3)	80(4)	7(3)	22(3)	5(3)
C(302)	186(11)	111(7)	227(14)	-50(8)	137(10)	-68(7)
C(303)	150(10)	134(9)	285(17)	-94(10)	91(11)	-89(8)
C(304)	237(13)	85(6)	122(8)	2(6)	69(9)	10(8)
C(305)	127(8)	163(11)	182(12)	-29(9)	75(8)	-11(7)
C(307)	186(11)	128(8)	110(8)	-33(6)	-3(7)	-42(7)
C(308)	89(6)	144(8)	123(8)	-5(6)	5(5)	-14(5)
Na(1B)	31(1)	30(1)	36(1)	-1(1)	6(1)	4(1)
O(1B)	31(1)	27(1)	28(2)	0(1)	9(1)	2(1)
C(1B)	26(2)	26(2)	27(2)	-3(2)	5(2)	0(2)
Na(2B)	32(1)	33(1)	34(1)	-1(1)	5(1)	3(1)
O(2B)	25(1)	33(2)	31(2)	0(1)	5(1)	6(1)
C(2B)	30(2)	32(2)	28(2)	1(2)	5(2)	2(2)
Na(3B)	33(1)	34(1)	35(1)	0(1)	7(1)	3(1)
O(3B)	27(1)	32(2)	32(2)	-6(1)	4(1)	5(1)
C(3B)	30(2)	30(2)	29(2)	2(2)	5(2)	-2(2)
C(4B)	41(2)	35(2)	36(2)	6(2)	9(2)	-2(2)
C(5B)	72(3)	32(2)	50(3)	15(2)	20(3)	1(2)
C(6B)	79(4)	35(3)	80(4)	-6(3)	29(3)	-12(3)
C(7B)	121(5)	42(3)	82(4)	31(3)	51(4)	10(3)
C(8B)	66(3)	50(3)	66(4)	22(3)	16(3)	22(3)
C(9B)	60(3)	47(3)	40(3)	12(2)	20(2)	-2(2)
C(10B)	58(3)	52(3)	33(3)	-1(2)	16(2)	0(2)
C(11B)	104(5)	76(4)	42(3)	7(3)	38(3)	5(4)
C(12C)	88(11)	150(16)	94(12)	-52(11)	79(10)	-57(11)
C(12D)	90(12)	168(19)	82(11)	-28(12)	50(9)	5(12)
C(13C)	110(13)	106(12)	40(8)	-7(8)	38(8)	26(11)
C(13D)	150(19)	108(14)	46(9)	-25(9)	12(10)	4(13)
C(14C)	115(12)	135(13)	13(5)	4(6)	13(6)	36(10)
C(15B)	46(3)	37(2)	31(2)	-1(2)	12(2)	4(2)
C(16B)	24(2)	21(2)	32(2)	-3(2)	2(2)	-1(2)
C(17B)	24(2)	23(2)	37(2)	-2(2)	5(2)	1(2)
C(18B)	31(2)	30(2)	37(2)	-2(2)	-1(2)	5(2)
C(19B)	35(2)	59(3)	39(3)	5(2)	-5(2)	10(2)

C(20B)	45(3)	78(4)	38(3)	-10(3)	-6(2)	11(3)
C(21B)	57(3)	72(4)	45(3)	23(3)	2(2)	9(3)
C(22B)	46(3)	94(4)	50(3)	7(3)	-14(2)	22(3)
C(23B)	23(2)	39(2)	58(3)	-4(2)	-1(2)	8(2)
C(24B)	27(2)	39(2)	47(3)	-11(2)	5(2)	1(2)
C(25B)	26(2)	69(3)	65(3)	-19(3)	15(2)	3(2)
C(26B)	29(3)	133(6)	79(4)	-27(4)	10(3)	-10(3)
C(27B)	39(3)	153(7)	74(4)	-40(4)	26(3)	-3(4)
C(28B)	75(5)	83(5)	177(9)	-20(5)	59(5)	33(4)
C(29B)	33(2)	34(2)	36(2)	-7(2)	7(2)	-2(2)
C(30B)	30(2)	29(2)	23(2)	-2(2)	2(2)	4(2)
C(31B)	30(2)	24(2)	25(2)	-4(2)	4(2)	4(2)
C(32B)	31(2)	36(2)	38(2)	-8(2)	-1(2)	2(2)
C(33B)	30(2)	48(3)	66(3)	-23(2)	-4(2)	-2(2)
C(34B)	40(3)	50(3)	82(4)	-19(3)	22(3)	-12(2)
C(35B)	36(3)	80(4)	79(4)	-28(3)	-17(3)	14(3)
C(36B)	40(3)	74(4)	107(5)	-53(4)	1(3)	-10(3)
C(37B)	34(2)	34(2)	39(2)	-12(2)	-1(2)	1(2)
C(38B)	36(2)	33(2)	33(2)	-7(2)	5(2)	6(2)
C(39B)	39(2)	37(2)	47(3)	-16(2)	7(2)	6(2)
C(40B)	46(3)	55(3)	95(4)	-36(3)	16(3)	7(2)
C(41B)	77(4)	67(4)	58(3)	-22(3)	11(3)	15(3)
C(42B)	63(3)	40(3)	82(4)	-16(3)	16(3)	11(2)
C(43B)	29(2)	30(2)	31(2)	-3(2)	3(2)	5(2)
O(401)	46(2)	72(3)	138(4)	-28(3)	26(3)	-13(2)
C(401)	44(3)	53(3)	96(5)	0(3)	18(3)	-4(3)
C(402)	83(5)	108(6)	160(9)	18(6)	-24(6)	-28(5)
C(403)	119(8)	107(7)	236(14)	19(8)	-98(9)	-34(6)
C(404)	79(5)	109(7)	193(11)	44(7)	17(6)	-18(5)
C(405)	160(10)	117(8)	155(10)	36(7)	-22(8)	-59(7)
C(406)	125(7)	108(7)	132(8)	18(6)	-17(6)	-40(6)
C(407)	92(6)	132(7)	124(8)	36(6)	-11(5)	-7(5)
C(408)	140(8)	104(6)	96(6)	-11(5)	3(6)	-37(6)
O(501)	131(4)	54(3)	85(3)	0(2)	22(3)	24(3)
C(501)	91(5)	73(4)	59(4)	-2(3)	5(3)	36(4)
C(502)	101(5)	73(5)	89(5)	-5(4)	9(4)	-1(4)
C(503)	130(7)	82(5)	109(7)	10(5)	1(5)	-4(5)
C(504)	143(8)	73(5)	115(7)	26(5)	0(6)	7(5)
C(505)	125(7)	88(5)	85(5)	11(4)	12(5)	36(5)
C(506)	88(5)	64(4)	72(4)	-8(3)	2(3)	15(3)
C(507)	131(7)	109(7)	106(7)	-5(5)	4(6)	-15(5)
C(508)	120(6)	64(4)	101(6)	-6(4)	22(5)	-5(4)
O(601)	61(4)	108(5)	19(3)	0(3)	5(3)	-9(3)
C(601)	52(5)	52(5)	52(6)	6(4)	6(4)	12(4)
C(603)	193(18)	131(13)	210(20)	37(13)	-165(17)	3(12)
C(608)	111(9)	72(7)	80(8)	7(6)	-4(7)	35(7)

Table 48. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3a·5.6$C_8H_{14}O$** (2,6-dimethyl cyclohexanone).

	x	y	z	U(eq)
H(1A)	4668	5547	4410	32
H(6A)	5057	6535	6187	88
H(6B)	4859	7123	6210	88
H(6C)	5372	6949	6598	88
H(7A)	5862	7669	6149	103
H(7B)	5363	7837	5731	103

H(7C)	5917	7722	5430	103
H(8A)	5959	6340	5674	84
H(8B)	6235	6780	6084	84
H(8C)	6263	6807	5361	84
H(9A)	5250	7670	4733	53
H(12A)	5500	8120	3871	169
H(12B)	5263	8334	3238	169
H(12C)	5554	7785	3265	169
H(12D)	5295	8362	3926	168
H(12E)	4822	8263	4375	168
H(12F)	4715	8569	3752	168
H(13A)	4777	7419	2712	167
H(13B)	4357	7878	2762	167
H(13C)	4232	7321	3040	167
H(13D)	5467	7788	3181	112
H(13E)	4963	7924	2754	112
H(13F)	5086	7335	2935	112
H(14A)	4653	8312	4264	153
H(14B)	4134	7984	4095	153
H(14C)	4331	8422	3641	153
H(14D)	3931	7812	3751	195
H(14E)	4050	7429	3201	195
H(14F)	4082	8042	3105	195
H(15A)	4540	6719	3507	45
H(20A)	2889	4581	5869	84
H(20B)	2907	5200	5852	84
H(20C)	3416	4872	5679	84
H(21A)	2820	4063	4930	93
H(21B)	3347	4304	4667	93
H(21C)	2807	4329	4274	93
H(22A)	2066	4616	5165	113
H(22B)	2082	4943	4549	113
H(22C)	2115	5233	5190	113
H(23A)	2413	5720	4410	47
H(26A)	2074	6609	3036	125
H(26B)	2103	6055	3361	125
H(26C)	2561	6231	2922	125
H(27A)	1987	7050	4041	114
H(27B)	2420	6966	4576	114
H(27C)	2020	6508	4393	114
H(28A)	2677	7325	3375	125
H(28B)	3141	6944	3186	125
H(28C)	3156	7206	3844	125
H(29A)	3701	6481	3824	40
H(34A)	5775	4953	1724	104
H(34B)	5347	4497	1721	104
H(34C)	5958	4368	1843	104
H(35A)	5693	3897	2779	85
H(35B)	5089	4064	2679	85
H(35C)	5394	4189	3308	85
H(36A)	6292	5163	2702	82
H(36B)	6412	4565	2836	82
H(36C)	6128	4911	3332	82
H(37A)	4984	5280	1861	44
H(40A)	3701	5311	1566	111
H(40B)	4247	5310	1223	111
H(40C)	3779	5684	996	111
H(41A)	3447	6084	2204	91
H(41B)	3512	6437	1615	91
H(41C)	3820	6584	2236	91
H(42A)	4667	6613	1705	116
H(42B)	4388	6453	1071	116
H(42C)	4876	6123	1340	116

H(43A)	4063	6056	3022	42
H(10A)	3060	6119	6689	128
H(10B)	3331	6835	7200	211
H(10C)	2706	6775	7274	211
H(10D)	2545	7424	6444	162
H(10E)	2896	7688	6979	162
H(10F)	3313	7847	6035	161
H(10G)	3689	7485	6449	161
H(10H)	3002	7139	5514	96
H(10I)	2122	6285	6437	254
H(10J)	2410	6124	5829	254
H(10K)	2278	6719	5957	254
H(10L)	3772	7595	5173	118
H(10M)	3686	7028	4893	118
H(10N)	4117	7119	5429	118
H(20D)	4101	3723	2671	246
H(20E)	3506	3190	2038	209
H(20F)	3384	3221	2751	209
H(20G)	2626	3419	2209	246
H(20Q)	2929	3817	1800	246
H(20H)	2344	4306	2379	225
H(20I)	2567	4052	3006	225
H(20J)	3138	4610	2168	294
H(20K)	3848	3861	1491	337
H(20L)	4397	4003	1829	337
H(20M)	3940	4428	1768	337
H(20N)	2603	5180	2700	213
H(20O)	3187	5266	2977	213
H(20P)	2772	4930	3342	213
H(30A)	6415	7236	3288	206
H(30B)	7396	7213	3185	225
H(30C)	7400	6623	3431	225
H(30D)	6709	6953	2415	176
H(30E)	7263	6683	2296	176
H(30F)	6954	5952	2817	187
H(30G)	6649	6072	2182	187
H(30H)	6040	5921	3045	167
H(30I)	6376	7398	4327	213
H(30J)	6931	7602	4097	213
H(30K)	6901	7067	4462	213
H(30L)	5434	6490	2820	178
H(30M)	5731	6350	2213	178
H(30N)	5854	6885	2554	178
H(1BA)	-534	10296	-4383	31
H(6BA)	-753	7909	-4012	96
H(6BB)	-804	8475	-4305	96
H(6BC)	-1269	8251	-3906	96
H(7BA)	-644	7782	-2906	121
H(7BB)	-1148	8135	-2782	121
H(7BC)	-593	8264	-2451	121
H(8BA)	107	8126	-3510	90
H(8BB)	159	8586	-3025	90
H(8BC)	108	8715	-3735	90
H(9BA)	-1111	8964	-2445	59
H(12G)	-2208	9602	-2256	164
H(12H)	-2100	9565	-1537	164
H(12I)	-1832	9157	-1979	164
H(12J)	-2072	10388	-2349	168
H(12K)	-2270	10069	-1777	168
H(12L)	-2237	9793	-2424	168
H(13G)	-1792	10574	-2237	127
H(13H)	-1226	10628	-1901	127
H(13I)	-1735	10502	-1516	127

H(13J)	-1247	10643	-1946	151
H(13K)	-854	10271	-1566	151
H(13L)	-1416	10419	-1303	151
H(14G)	-729	9798	-1444	132
H(14H)	-1055	9268	-1456	132
H(14I)	-1232	9734	-1030	132
H(14J)	-1747	9155	-1741	204
H(14K)	-1646	9531	-1172	204
H(14L)	-1158	9263	-1490	204
H(15B)	-1173	10469	-2948	45
H(20R)	-1320	10162	-6335	81
H(20S)	-1700	10307	-6903	81
H(20T)	-1936	10028	-6323	81
H(21D)	-1037	11157	-6203	87
H(21E)	-1500	11577	-6249	87
H(21F)	-1374	11226	-6824	87
H(22D)	-2440	11330	-6246	96
H(22E)	-2610	10735	-6316	96
H(22F)	-2339	11028	-6866	96
H(23B)	-2535	10978	-5343	48
H(26D)	-3278	10726	-4864	120
H(26E)	-3573	10796	-4237	120
H(26F)	-3206	10302	-4339	120
H(27D)	-3069	10945	-3274	132
H(27E)	-2454	11087	-3270	132
H(27F)	-2641	10502	-3384	132
H(28D)	-2902	11645	-4684	165
H(28E)	-2557	11759	-4078	165
H(28F)	-3180	11674	-4043	165
H(29B)	-1790	10614	-3741	41
H(34D)	931	11393	-4554	86
H(34E)	1400	11772	-4340	86
H(34F)	816	11995	-4449	86
H(35D)	1137	10807	-3607	98
H(35E)	1194	11079	-2956	98
H(35F)	1617	11195	-3463	98
H(36D)	1460	12132	-3288	111
H(36E)	996	12032	-2827	111
H(36F)	891	12385	-3415	111
H(37B)	128	12093	-3040	43
H(40D)	-1599	11682	-2720	97
H(40E)	-1632	12055	-3300	97
H(40F)	-1711	12288	-2636	97
H(41D)	-846	11752	-1970	100
H(41E)	-898	12366	-1896	100
H(41F)	-352	12118	-2093	100
H(42D)	-1019	12948	-2760	92
H(42E)	-929	12753	-3438	92
H(42F)	-440	12793	-2963	92
H(43B)	-1184	11267	-3477	36
H(40G)	-3010	9394	-4780	141
H(40H)	-3335	8601	-5327	187
H(40I)	-2732	8444	-5446	187
H(40J)	-3050	8057	-4520	152
H(40K)	-3126	8627	-4252	152
H(40L)	-2115	8212	-4559	173
H(40M)	-2318	8242	-3877	173
H(40N)	-1734	8960	-4166	147
H(40O)	-2775	9898	-5627	174
H(40P)	-3271	9536	-5792	174
H(40Q)	-2697	9381	-6014	174
H(40R)	-2215	9647	-3756	170
H(40S)	-2158	9145	-3334	170

H(40T)	-2700	9256	-3701	170
H(50A)	324	12656	-5122	105
H(50B)	38	13518	-5482	128
H(50C)	-169	13053	-5908	128
H(50D)	-809	13592	-5037	132
H(50E)	-891	13630	-5760	132
H(50F)	-1144	12754	-5814	119
H(50G)	-1514	13048	-5351	119
H(50H)	-1009	12720	-4516	90
H(50I)	164	12799	-4058	173
H(50J)	-241	13250	-4243	173
H(50K)	372	13312	-4379	173
H(50L)	-1294	11862	-4502	142
H(50M)	-1339	11837	-5228	142
H(50N)	-1742	12186	-4861	142
H(60N)	278	9706	-1479	178
H(60A)	1375	9698	-1417	218
H(60B)	979	9603	-872	218
H(60C)	633	10463	-983	283
H(60D)	1261	10506	-893	283
H(60E)	1341	10590	-1962	303
H(60F)	993	11049	-1695	303
H(60G)	629	10653	-2644	177
H(60H)	218	8974	-1598	219
H(60I)	843	8928	-1494	219
H(60J)	593	8973	-2168	219
H(60K)	-189	10808	-2416	131
H(60L)	145	11144	-1930	131
H(60M)	-108	10604	-1734	131
H(80C)	5734	5978	279	174
H(80D)	5157	5973	-36	174
H(80E)	5655	5792	-411	174
H(80A)	5735	5142	-2	90
H(80B)	5520	5348	613	90
H(80G)	5699	6090	184	221
H(80H)	5980	5539	118	221
H(80I)	5654	5666	709	221
H(80F)	4817	5688	38	127
H(80J)	5163	5480	-514	127
H(90E)	-1526	6320	-5277	183
H(90F)	-1192	6844	-5209	183
H(90G)	-1823	6864	-5228	183
H(90S)	-1604	6253	-4499	111
H(90T)	-1134	6649	-4440	111
H(90D)	-1702	6589	-3426	91
H(90M)	-1452	7138	-3528	91
H(90I)	-1333	6590	-5571	116
H(90J)	-1698	7095	-5592	116
H(90K)	-1960	6533	-5548	116

Table 49. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ***trans*-2,6-dimethylcyclohexanone 2,4-dinitrophenylhydrazone**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	1981(1)	3167(3)	570(1)	28(1)
C(1)	2849(2)	3357(3)	729(2)	27(1)
O(1)	977(1)	1497(3)	-2109(1)	57(1)
N(2)	1392(1)	2618(3)	-346(2)	31(1)
C(2)	3279(2)	3056(4)	-2(2)	35(1)
O(2)	-440(1)	910(3)	-3032(1)	52(1)
C(3)	4246(2)	2103(4)	449(2)	44(1)
N(3)	146(2)	1366(3)	-2245(2)	36(1)
O(3)	-2918(1)	1038(3)	-2000(2)	47(1)
C(4)	4866(2)	3035(4)	1387(2)	44(1)
O(4)	-2643(1)	1431(3)	-496(2)	46(1)
N(4)	-2388(2)	1367(3)	-1168(2)	36(1)
C(5)	4397(2)	2960(4)	2093(2)	40(1)
C(6)	3471(2)	4063(4)	1719(2)	31(1)
C(7)	3297(2)	4979(4)	-496(2)	49(1)
C(8)	3005(2)	4023(4)	2434(2)	38(1)
C(10)	485(2)	2331(3)	-550(2)	25(1)
C(11)	-151(2)	1724(3)	-1474(2)	27(1)
C(12)	-1089(2)	1430(3)	-1668(2)	29(1)
C(13)	-1407(2)	1710(3)	-961(2)	28(1)
C(14)	-813(2)	2308(3)	-51(2)	27(1)
C(15)	107(2)	2621(3)	150(2)	26(1)

Table 50. Bond lengths [A] and angles [deg] for ***trans*-2,6-dimethylcyclohexanone 2,4-dinitrophenylhydrazone**.

N(1)-C(1)	1.286(3)	C(4)-C(5)	1.516(4)
N(1)-N(2)	1.385(3)	O(4)-N(4)	1.231(3)
C(1)-C(6)	1.514(4)	N(4)-C(13)	1.456(3)
C(1)-C(2)	1.517(3)	C(5)-C(6)	1.531(3)
O(1)-N(3)	1.233(3)	C(6)-C(8)	1.525(3)
N(2)-C(10)	1.341(3)	C(10)-C(15)	1.415(3)
C(2)-C(7)	1.526(4)	C(10)-C(11)	1.426(3)
C(2)-C(3)	1.538(3)	C(11)-C(12)	1.391(3)
O(2)-N(3)	1.227(3)	C(12)-C(13)	1.362(3)
C(3)-C(4)	1.514(4)	C(13)-C(14)	1.390(3)
N(3)-C(11)	1.438(3)	C(14)-C(15)	1.365(3)
O(3)-N(4)	1.230(3)		

C(1)-N(1)-N(2)	116.9(2)	C(4)-C(5)-C(6)	111.6(2)
N(1)-C(1)-C(6)	115.9(2)	C(1)-C(6)-C(8)	113.6(2)
N(1)-C(1)-C(2)	125.8(2)	C(1)-C(6)-C(5)	110.8(2)
C(6)-C(1)-C(2)	118.2(2)	C(8)-C(6)-C(5)	111.9(2)
C(10)-N(2)-N(1)	119.9(2)	N(2)-C(10)-C(15)	121.2(2)
C(1)-C(2)-C(7)	109.8(2)	N(2)-C(10)-C(11)	122.4(2)
C(1)-C(2)-C(3)	111.8(2)	C(15)-C(10)-C(11)	116.4(2)
C(7)-C(2)-C(3)	112.6(2)	C(12)-C(11)-C(10)	121.4(2)
C(4)-C(3)-C(2)	113.1(2)	C(12)-C(11)-N(3)	116.8(2)
O(2)-N(3)-O(1)	121.0(2)	C(10)-C(11)-N(3)	121.9(2)
O(2)-N(3)-C(11)	118.7(2)	C(13)-C(12)-C(11)	119.4(2)
O(1)-N(3)-C(11)	120.2(2)	C(12)-C(13)-C(14)	121.1(2)

C(3)-C(4)-C(5)	110.0(2)	C(12)-C(13)-N(4)	119.0(2)
O(3)-N(4)-O(4)	123.4(2)	C(14)-C(13)-N(4)	119.9(2)
O(3)-N(4)-C(13)	118.7(2)	C(15)-C(14)-C(13)	120.2(2)
O(4)-N(4)-C(13)	118.0(2)	C(14)-C(15)-C(10)	121.5(2)

Table 51. Anisotropic displacement parameters (A^2 x 10^3) for ***trans*-2,6-dimethylcyclohexanone 2,4-dinitrophenylhydrazone**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	26(1)	32(1)	23(1)	0(1)	7(1)	0(1)
C(1)	25(1)	26(1)	32(2)	1(1)	13(1)	-1(1)
O(1)	38(1)	97(2)	41(1)	-17(1)	22(1)	-7(1)
N(2)	25(1)	42(1)	26(1)	-1(1)	11(1)	-1(1)
C(2)	28(1)	42(2)	36(2)	-8(1)	13(1)	-5(1)
O(2)	50(1)	75(2)	25(1)	-7(1)	9(1)	-6(1)
C(3)	32(2)	47(2)	58(2)	-9(2)	22(2)	-2(1)
N(3)	39(1)	41(1)	28(1)	1(1)	13(1)	1(1)
O(3)	27(1)	49(1)	50(1)	-2(1)	0(1)	-4(1)
C(4)	24(1)	50(2)	53(2)	-1(2)	10(1)	1(1)
O(4)	32(1)	50(1)	60(2)	-2(1)	23(1)	-3(1)
N(4)	27(1)	28(1)	50(2)	3(1)	11(1)	0(1)
C(5)	28(2)	41(2)	43(2)	3(1)	5(1)	-4(1)
C(6)	28(1)	30(1)	32(2)	0(1)	10(1)	-3(1)
C(7)	49(2)	65(2)	41(2)	6(2)	27(2)	1(2)
C(8)	36(2)	44(2)	30(2)	-2(1)	10(1)	-5(1)
C(10)	25(1)	24(1)	24(1)	4(1)	8(1)	3(1)
C(11)	31(1)	27(1)	24(1)	2(1)	12(1)	2(1)
C(12)	28(1)	27(1)	24(1)	0(1)	1(1)	0(1)
C(13)	21(1)	24(1)	35(2)	3(1)	8(1)	2(1)
C(14)	29(1)	24(1)	31(2)	2(1)	14(1)	2(1)
C(15)	26(1)	24(1)	24(1)	1(1)	7(1)	1(1)

Table 52. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ***trans*-2,6-dimethylcyclohexanone 2,4-dinitrophenylhydrazone**.

	x	y	z	U(eq)
H(2A)	1599(18)	2390(40)	-780(20)	44(9)
H(2B)	2874	2165	-491	42
H(3A)	4170	735	558	53
H(3B)	4548	2189	0	53
H(4A)	4988	4376	1276	53
H(4B)	5456	2352	1650	53
H(5A)	4808	3524	2697	48
H(5B)	4287	1615	2209	48
H(6A)	3617	5426	1651	37
H(7A)	2684	5531	-751	74
H(7B)	3503	4754	-1007	74
H(7C)	3718	5862	-40	74

H(8A)	2447	4791	2192	57
H(8B)	3422	4546	3035	57
H(8C)	2851	2706	2524	57
H(12A)	-1495	1045	-2276	35
H(14A)	-1044	2494	423	33
H(15A)	495	3034	759	31

Table 53. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3a·6$C_5H_{14}O_2$** (2,2,6-Trimethylcyclo-hexyl-1,4-dione).
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)	site occupancy
Na(1)	1151(1)	-782(1)	22(1)	29(1)	
Na(2)	-924(1)	-1191(1)	114(1)	28(1)	
Na(3)	-37(1)	875(1)	854(1)	27(1)	
O(1)	1024(1)	312(1)	630(1)	26(1)	
O(2)	156(1)	-1604(1)	-66(1)	25(1)	
O(3)	-948(1)	-15(1)	724(1)	25(1)	
C(1)	185(1)	-1054(2)	1031(1)	23(1)	
C(2)	711(1)	-568(2)	1374(1)	23(1)	
C(3)	1139(1)	53(2)	1137(1)	24(1)	
C(4)	1679(1)	398(2)	1462(1)	27(1)	
C(5)	2171(2)	1066(2)	1231(1)	33(1)	
C(6)	2482(2)	735(2)	711(1)	41(1)	
C(7)	2763(2)	1257(2)	1620(1)	44(1)	
C(8)	1801(2)	1919(2)	1118(1)	38(1)	
C(9)	1520(2)	2370(2)	1606(1)	47(1)	
C(10)	1738(2)	140(2)	1996(1)	29(1)	
C(11)	1300(2)	-425(2)	2244(1)	28(1)	
C(12)	1392(2)	-666(2)	2844(1)	33(1)	
C(13)	1429(2)	169(3)	3181(1)	52(1)	
C(14)	2052(2)	-1153(2)	2918(1)	48(1)	
C(15)	808(2)	-1232(3)	3029(1)	52(1)	
C(16)	814(3)	-1477(4)	3628(2)	79(2)	
C(17)	789(1)	-764(2)	1921(1)	26(1)	
C(18)	453(1)	-1935(2)	846(1)	25(1)	
C(19)	392(1)	-2168(2)	297(1)	25(1)	
C(20)	611(2)	-3018(2)	145(1)	27(1)	
C(21)	583(2)	-3317(2)	-447(1)	31(1)	
C(22)	1079(2)	-2784(2)	-775(1)	39(1)	
C(23)	788(2)	-4266(2)	-513(1)	43(1)	
C(24)	-131(2)	-3215(2)	-697(1)	31(1)	
C(25)	-686(2)	-3626(2)	-384(1)	45(1)	
C(26)	860(2)	-3565(2)	545(1)	32(1)	
C(27)	940(2)	-3331(2)	1082(1)	32(1)	
C(28)	1177(2)	-3987(2)	1504(1)	41(1)	
C(29)	1419(4)	-3567(3)	2012(2)	98(2)	
C(30)	1733(3)	-4555(4)	1291(2)	91(2)	
C(31A)	574(7)	-4632(6)	1579(3)	68(3)	0.7
C(32A)	614(6)	-5229(5)	2034(3)	102(3)	0.7
C(31B)	603(12)	-4300(19)	1809(15)	135(13)	0.3
C(32B)	5(7)	-4593(8)	1738(5)	45(3)	0.3
C(33)	743(2)	-2504(2)	1216(1)	29(1)	
C(34)	-504(1)	-1114(2)	1304(1)	24(1)	
C(35)	-1029(1)	-534(2)	1147(1)	24(1)	

C(36)	-1637(2)	-551(2)	1448(1)	31(1)	
C(37)	-2230(2)	49(2)	1309(1)	38(1)	
C(38)	-2802(2)	-34(3)	1721(2)	69(1)	
C(39)	-2001(2)	989(2)	1332(2)	44(1)	
C(40)	-2512(2)	-185(3)	748(2)	54(1)	
C(41)	-3148(3)	240(5)	576(3)	111(2)	
C(42)	-1690(2)	-1132(2)	1868(1)	36(1)	
C(43)	-1192(2)	-1727(2)	2013(1)	36(1)	
C(44)	-1295(2)	-2319(2)	2502(1)	49(1)	
C(45)	-770(3)	-3035(3)	2516(2)	89(2)	
C(46)	-1986(2)	-2742(3)	2476(2)	65(1)	
C(47)	-1222(3)	-1750(4)	3004(2)	83(2)	
C(48)	-1325(5)	-2174(5)	3556(2)	135(3)	
C(49)	-612(2)	-1715(2)	1715(1)	31(1)	
O(101)	2094(1)	-1603(2)	131(1)	65(1)	
O(102)	4059(2)	-2837(2)	1330(1)	86(1)	
C(101)	2459(2)	-2016(3)	438(2)	62(1)	
C(102)	2853(3)	-2784(4)	259(2)	86(2)	
C(103)	3566(2)	-2790(3)	460(2)	64(1)	
C(104)	3635(2)	-2555(3)	1045(2)	56(1)	
C(105)	3211(3)	-1784(6)	1242(2)	128(3)	
C(106)	2509(2)	-1825(3)	1020(2)	64(1)	
C(107)	3921(3)	-3634(4)	333(2)	99(2)	
C(108)	3935(4)	-2090(5)	135(2)	127(3)	
C(109)	3229(4)	-1709(8)	1850(2)	181(5)	
O(201)	-1634(1)	-2258(2)	369(1)	54(1)	
O(202)	-3002(2)	-5095(2)	661(1)	84(1)	
C(201)	-2017(2)	-2797(2)	539(1)	45(1)	
C(202)	-2745(2)	-2813(3)	393(2)	52(1)	
C(203)	-2994(2)	-3715(3)	243(1)	56(1)	
C(204)	-2803(2)	-4362(3)	683(2)	52(1)	
C(205)	-2347(2)	-4054(2)	1136(1)	48(1)	
C(206)	-1780(2)	-3497(3)	916(1)	50(1)	
C(207)	-3762(2)	-3714(4)	157(2)	78(2)	
C(208)	-2658(3)	-4023(3)	-276(2)	78(2)	
C(209)	-2095(2)	-4779(3)	1500(2)	64(1)	
O(301)	-110(1)	1535(2)	1659(1)	50(1)	
O(302)	-1264(2)	2114(2)	3468(1)	86(1)	
C(301)	-183(2)	1631(2)	2138(1)	39(1)	
C(302)	-24(2)	2458(3)	2427(2)	52(1)	
C(303)	-593(2)	2741(2)	2793(1)	48(1)	
C(304)	-821(2)	2008(3)	3144(2)	53(1)	
C(305)	-476(2)	1147(3)	3076(2)	59(1)	
C(306)	-436(2)	912(3)	2485(2)	55(1)	
C(307)	-374(2)	3490(3)	3142(2)	69(1)	
C(308)	-1202(2)	3032(3)	2425(2)	74(1)	
C(309)	-736(4)	453(3)	3429(2)	101(2)	
O(401)	-5000	0	0	157(7)	0.2
C(401)	-5090(20)	120(30)	522(19)	133(14)	0.2
C(402)	-5380(20)	930(30)	628(18)	115(11)	0.2
C(404)	-5340(19)	540(30)	895(14)	105(10)	0.2
C(403)	-5310(20)	500(30)	353(14)	107(11)	0.2

Table 54. Bond lengths [A] and angles [deg] for **3a·6C$_9$H$_{14}$O$_2$** (2,2,6-Trimethylcyclo-hexyl-1,4-dione).

Na(1)-O(3)#1	2.261(2)	C(26)-C(27)	1.392(4)
Na(1)-O(101)	2.282(3)	C(27)-C(33)	1.385(4)
Na(1)-O(1)	2.293(2)	C(27)-C(28)	1.532(4)
Na(1)-O(2)	2.363(2)	C(28)-C(31B)	1.47(3)
Na(1)-C(19)	2.724(3)	C(28)-C(29)	1.494(5)
Na(1)-C(3)	3.063(3)	C(28)-C(30)	1.519(6)
Na(1)-C(18)	3.073(3)	C(28)-C(31A)	1.577(12)
Na(1)-Na(3)#1	3.0826(15)	C(31A)-C(32A)	1.465(11)
Na(1)-Na(2)#1	3.1149(15)	C(31B)-C(32B)	1.28(3)
Na(1)-Na(3)	4.0844(16)	C(34)-C(49)	1.403(4)
Na(1)-Na(2)	4.1902(16)	C(34)-C(35)	1.429(4)
Na(2)-O(201)	2.275(3)	C(35)-C(36)	1.437(4)
Na(2)-O(2)	2.297(2)	C(36)-C(42)	1.385(4)
Na(2)-O(1)#1	2.306(2)	C(36)-C(37)	1.538(4)
Na(2)-O(3)	2.376(2)	C(37)-C(39)	1.528(5)
Na(2)-C(35)	2.775(3)	C(37)-C(40)	1.540(5)
Na(2)-C(19)	3.054(3)	C(37)-C(38)	1.551(5)
Na(2)-C(34)	3.062(3)	C(40)-C(41)	1.485(7)
Na(2)-Na(1)#1	3.1149(15)	C(42)-C(43)	1.397(5)
Na(2)-Na(3)#1	3.1422(15)	C(43)-C(49)	1.385(4)
Na(2)-Na(3)	4.0838(15)	C(43)-C(44)	1.542(4)
Na(3)-O(301)	2.257(2)	C(44)-C(46)	1.525(5)
Na(3)-O(2)#1	2.272(2)	C(44)-C(45)	1.526(6)
Na(3)-O(3)	2.297(2)	C(44)-C(47)	1.535(6)
Na(3)-O(1)	2.362(2)	C(47)-C(48)	1.539(6)
Na(3)-C(3)	2.748(3)	O(101)-C(101)	1.226(4)
Na(3)-C(2)	2.974(3)	O(102)-C(104)	1.178(4)
Na(3)-C(35)	3.043(3)	C(101)-C(106)	1.479(6)
Na(3)-C(1)	3.059(3)	C(101)-C(102)	1.500(6)
Na(3)-Na(1)#1	3.0826(15)	C(102)-C(103)	1.495(6)
Na(3)-Na(2)#1	3.1422(15)	C(103)-C(104)	1.504(6)
O(1)-C(3)	1.339(3)	C(103)-C(107)	1.523(7)
O(1)-Na(2)#1	2.306(2)	C(103)-C(108)	1.548(8)
O(2)-C(19)	1.336(3)	C(104)-C(105)	1.550(7)
O(2)-Na(3)#1	2.272(2)	C(105)-C(106)	1.496(7)
O(3)-C(35)	1.336(3)	C(105)-C(109)	1.514(7)
O(3)-Na(1)#1	2.261(2)	O(201)-C(201)	1.214(4)
C(1)-C(2)	1.536(4)	O(202)-C(204)	1.206(5)
C(1)-C(18)	1.541(4)	C(201)-C(202)	1.487(5)
C(1)-C(34)	1.544(4)	C(201)-C(206)	1.506(5)
C(2)-C(17)	1.399(4)	C(202)-C(203)	1.529(6)
C(2)-C(3)	1.422(4)	C(203)-C(204)	1.529(6)
C(3)-C(4)	1.436(4)	C(203)-C(207)	1.539(6)
C(4)-C(10)	1.391(4)	C(203)-C(208)	1.542(5)
C(4)-C(5)	1.546(4)	C(204)-C(205)	1.511(5)
C(5)-C(6)	1.534(5)	C(205)-C(209)	1.523(5)
C(5)-C(7)	1.539(4)	C(205)-C(206)	1.533(5)
C(5)-C(8)	1.539(4)	O(301)-C(301)	1.210(4)
C(8)-C(9)	1.516(5)	O(302)-C(304)	1.217(4)
C(10)-C(11)	1.389(4)	C(301)-C(302)	1.503(5)
C(11)-C(17)	1.389(4)	C(301)-C(306)	1.504(5)
C(11)-C(12)	1.547(4)	C(302)-C(303)	1.532(5)
C(12)-C(14)	1.524(5)	C(303)-C(304)	1.510(6)
C(12)-C(15)	1.536(5)	C(303)-C(307)	1.510(5)
C(12)-C(13)	1.543(5)	C(303)-C(308)	1.573(6)
C(15)-C(16)	1.537(5)	C(304)-C(305)	1.514(6)
C(18)-C(33)	1.393(4)	C(305)-C(309)	1.488(6)
C(18)-C(19)	1.418(4)	C(305)-C(306)	1.518(5)
C(19)-C(20)	1.443(4)	O(401)-C(401)	1.33(5)

C(20)-C(26)	1.392(4)	O(401)-C(401)#2	1.33(5)
C(20)-C(21)	1.542(4)	O(401)-C(403)#2	1.34(4)
C(21)-C(22)	1.536(4)	O(401)-C(403)	1.34(4)
C(21)-C(23)	1.539(4)	C(401)-C(402)	1.40(6)
C(21)-C(24)	1.549(4)	C(404)-C(403)	1.35(5)
C(24)-C(25)	1.505(5)		

O(3)#1-Na(1)-O(101)	122.51(10)	C(35)-O(3)-Na(2)	92.45(15)
O(3)#1-Na(1)-O(1)	96.66(8)	Na(1)#1-O(3)-Na(2)	84.38(7)
O(101)-Na(1)-O(1)	115.86(10)	Na(3)-O(3)-Na(2)	121.83(9)
O(3)#1-Na(1)-O(2)	94.75(7)	C(2)-C(1)-C(18)	111.5(2)
O(101)-Na(1)-O(2)	113.34(10)	C(2)-C(1)-C(34)	112.8(2)
O(1)-Na(1)-O(2)	111.04(8)	C(18)-C(1)-C(34)	113.1(2)
O(3)#1-Na(1)-C(19)	123.14(8)	C(2)-C(1)-Na(3)	72.20(13)
O(101)-Na(1)-C(19)	89.35(10)	C(18)-C(1)-Na(3)	151.15(18)
O(1)-Na(1)-C(19)	110.57(9)	C(34)-C(1)-Na(3)	89.71(15)
O(2)-Na(1)-C(19)	29.36(7)	C(17)-C(2)-C(3)	119.6(2)
O(3)#1-Na(1)-C(3)	120.48(8)	C(17)-C(2)-C(1)	119.6(2)
O(101)-Na(1)-C(3)	98.56(10)	C(3)-C(2)-C(1)	120.7(2)
O(1)-Na(1)-C(3)	23.85(7)	C(17)-C(2)-Na(3)	129.24(19)
O(2)-Na(1)-C(3)	107.00(8)	C(3)-C(2)-Na(3)	66.94(14)
C(19)-Na(1)-C(3)	95.39(8)	C(1)-C(2)-Na(3)	78.34(14)
O(3)#1-Na(1)-C(18)	142.22(8)	O(1)-C(3)-C(2)	120.0(2)
O(101)-Na(1)-C(18)	88.68(10)	O(1)-C(3)-C(4)	122.1(2)
O(1)-Na(1)-C(18)	86.23(8)	C(2)-C(3)-C(4)	117.8(2)
O(2)-Na(1)-C(18)	50.11(7)	O(1)-C(3)-Na(3)	59.22(13)
C(19)-Na(1)-C(18)	27.47(8)	C(2)-C(3)-Na(3)	84.63(16)
C(3)-Na(1)-C(18)	68.37(7)	C(4)-C(3)-Na(3)	126.63(18)
O(3)#1-Na(1)-Na(3)#1	47.94(5)	O(1)-C(3)-Na(1)	43.84(12)
O(101)-Na(1)-Na(3)#1	129.61(9)	C(2)-C(3)-Na(1)	95.91(16)
O(1)-Na(1)-Na(3)#1	114.49(6)	C(4)-C(3)-Na(1)	130.53(19)
O(2)-Na(1)-Na(3)#1	47.06(5)	Na(3)-C(3)-Na(1)	89.15(8)
C(19)-Na(1)-Na(3)#1	75.24(6)	C(10)-C(4)-C(3)	118.7(3)
C(3)-Na(1)-Na(3)#1	129.98(7)	C(10)-C(4)-C(5)	120.3(2)
C(18)-Na(1)-Na(3)#1	96.68(6)	C(3)-C(4)-C(5)	120.9(2)
O(3)#1-Na(1)-Na(2)#1	49.38(5)	C(6)-C(5)-C(7)	106.1(3)
O(101)-Na(1)-Na(2)#1	132.80(9)	C(6)-C(5)-C(8)	109.5(3)
O(1)-Na(1)-Na(2)#1	47.55(5)	C(7)-C(5)-C(8)	107.9(3)
O(2)-Na(1)-Na(2)#1	113.70(6)	C(6)-C(5)-C(4)	110.9(2)
C(19)-Na(1)-Na(2)#1	136.42(7)	C(7)-C(5)-C(4)	112.3(2)
C(3)-Na(1)-Na(2)#1	71.23(6)	C(8)-C(5)-C(4)	109.9(3)
C(18)-Na(1)-Na(2)#1	125.38(7)	C(9)-C(8)-C(5)	115.7(3)
Na(3)#1-Na(1)-Na(2)#1	82.44(4)	C(11)-C(10)-C(4)	124.1(3)
O(3)#1-Na(1)-Na(3)	88.54(6)	C(10)-C(11)-C(17)	116.3(2)
O(101)-Na(1)-Na(3)	140.80(9)	C(10)-C(11)-C(12)	121.0(2)
O(1)-Na(1)-Na(3)	29.13(5)	C(17)-C(11)-C(12)	122.7(3)
O(2)-Na(1)-Na(3)	83.97(6)	C(14)-C(12)-C(15)	109.6(3)
C(19)-Na(1)-Na(3)	92.37(7)	C(14)-C(12)-C(13)	108.6(3)
C(3)-Na(1)-Na(3)	42.28(5)	C(15)-C(12)-C(13)	110.2(3)
C(18)-Na(1)-Na(3)	75.86(6)	C(14)-C(12)-C(11)	108.9(3)
Na(3)#1-Na(1)-Na(3)	88.39(4)	C(15)-C(12)-C(11)	110.5(2)
Na(2)#1-Na(1)-Na(3)	49.54(3)	C(13)-C(12)-C(11)	108.9(3)
O(3)#1-Na(1)-Na(2)	88.07(6)	C(12)-C(15)-C(16)	116.1(3)
O(101)-Na(1)-Na(2)	135.99(9)	C(11)-C(17)-C(2)	123.1(3)
O(1)-Na(1)-Na(2)	87.43(6)	C(33)-C(18)-C(19)	120.1(3)
O(2)-Na(1)-Na(2)	25.54(5)	C(33)-C(18)-C(1)	120.5(2)
C(19)-Na(1)-Na(2)	46.71(6)	C(19)-C(18)-C(1)	119.4(2)
C(3)-Na(1)-Na(2)	89.47(6)	C(33)-C(18)-Na(1)	128.5(2)
C(18)-Na(1)-Na(2)	54.33(5)	C(19)-C(18)-Na(1)	62.41(15)
Na(3)#1-Na(1)-Na(2)	48.30(3)	C(1)-C(18)-Na(1)	81.11(15)
Na(2)#1-Na(1)-Na(2)	90.80(4)	O(2)-C(19)-C(18)	120.5(2)
Na(3)-Na(1)-Na(2)	59.13(3)	O(2)-C(19)-C(20)	121.8(2)
O(201)-Na(2)-O(2)	116.12(10)	C(18)-C(19)-C(20)	117.7(2)

O(201)-Na(2)-O(1)#1	127.60(10)	O(2)-C(19)-Na(1)	60.16(13)
O(2)-Na(2)-O(1)#1	94.32(8)	C(18)-C(19)-Na(1)	90.12(17)
O(201)-Na(2)-O(3)	111.21(9)	C(20)-C(19)-Na(1)	119.01(19)
O(2)-Na(2)-O(3)	111.65(8)	O(2)-C(19)-Na(2)	44.34(12)
O(1)#1-Na(2)-O(3)	93.18(7)	C(18)-C(19)-Na(2)	94.30(17)
O(201)-Na(2)-C(35)	87.26(9)	C(20)-C(19)-Na(2)	132.74(19)
O(2)-Na(2)-C(35)	111.71(8)	Na(1)-C(19)-Na(2)	92.81(8)
O(1)#1-Na(2)-C(35)	121.23(8)	C(26)-C(20)-C(19)	118.5(2)
O(3)-Na(2)-C(35)	28.75(7)	C(26)-C(20)-C(21)	120.3(2)
O(201)-Na(2)-C(19)	97.64(10)	C(19)-C(20)-C(21)	121.2(2)
O(2)-Na(2)-C(19)	23.98(7)	C(22)-C(21)-C(23)	106.5(3)
O(1)#1-Na(2)-C(19)	118.29(8)	C(22)-C(21)-C(20)	109.5(2)
O(3)-Na(2)-C(19)	108.29(8)	C(23)-C(21)-C(20)	112.6(2)
C(35)-Na(2)-C(19)	97.13(8)	C(22)-C(21)-C(24)	109.0(2)
O(201)-Na(2)-C(34)	85.36(9)	C(23)-C(21)-C(24)	107.3(2)
O(2)-Na(2)-C(34)	87.66(8)	C(20)-C(21)-C(24)	111.7(2)
O(1)#1-Na(2)-C(34)	140.42(8)	C(25)-C(24)-C(21)	115.2(3)
O(3)-Na(2)-C(34)	50.29(7)	C(20)-C(26)-C(27)	124.1(3)
C(35)-Na(2)-C(34)	27.79(8)	C(33)-C(27)-C(26)	116.4(3)
C(19)-Na(2)-C(34)	69.96(8)	C(33)-C(27)-C(28)	122.5(3)
O(201)-Na(2)-Na(1)#1	131.06(9)	C(26)-C(27)-C(28)	120.9(3)
O(2)-Na(2)-Na(1)#1	112.82(6)	C(31B)-C(28)-C(29)	87.2(16)
O(1)#1-Na(2)-Na(1)#1	47.19(5)	C(31B)-C(28)-C(30)	124.7(13)
O(3)-Na(2)-Na(1)#1	46.25(5)	C(29)-C(28)-C(30)	108.9(4)
C(35)-Na(2)-Na(1)#1	74.05(6)	C(31B)-C(28)-C(27)	109.9(8)
C(19)-Na(2)-Na(1)#1	128.82(6)	C(29)-C(28)-C(27)	112.3(3)
C(34)-Na(2)-Na(1)#1	95.91(6)	C(30)-C(28)-C(27)	111.3(3)
O(201)-Na(2)-Na(3)#1	135.88(8)	C(31B)-C(28)-C(31A)	29.0(17)
O(2)-Na(2)-Na(3)#1	46.21(5)	C(29)-C(28)-C(31A)	114.4(4)
O(1)#1-Na(2)-Na(3)#1	48.45(6)	C(30)-C(28)-C(31A)	103.6(5)
O(3)-Na(2)-Na(3)#1	112.88(6)	C(27)-C(28)-C(31A)	106.0(4)
C(35)-Na(2)-Na(3)#1	135.13(7)	C(32A)-C(31A)-C(28)	117.5(8)
C(19)-Na(2)-Na(3)#1	70.02(6)	C(32B)-C(31B)-C(28)	141(3)
C(34)-Na(2)-Na(3)#1	125.08(7)	C(27)-C(33)-C(18)	123.1(3)
Na(1)#1-Na(2)-Na(3)#1	81.50(4)	C(49)-C(34)-C(35)	119.8(3)
O(201)-Na(2)-Na(3)	135.38(7)	C(49)-C(34)-C(1)	120.6(2)
O(2)-Na(2)-Na(3)	84.76(6)	C(35)-C(34)-C(1)	119.5(2)
O(1)#1-Na(2)-Na(3)	85.81(5)	C(49)-C(34)-Na(2)	129.41(18)
O(3)-Na(2)-Na(3)	28.55(5)	C(35)-C(34)-Na(2)	64.85(14)
C(35)-Na(2)-Na(3)	48.17(6)	C(1)-C(34)-Na(2)	78.93(14)
C(19)-Na(2)-Na(3)	87.74(6)	O(3)-C(35)-C(34)	119.8(2)
C(34)-Na(2)-Na(3)	54.95(5)	O(3)-C(35)-C(36)	122.5(2)
Na(1)#1-Na(2)-Na(3)	48.44(3)	C(34)-C(35)-C(36)	117.7(2)
Na(3)#1-Na(2)-Na(3)	87.60(3)	O(3)-C(35)-Na(2)	58.81(12)
O(201)-Na(2)-Na(1)	138.06(9)	C(34)-C(35)-Na(2)	87.36(16)
O(2)-Na(2)-Na(1)	26.33(5)	C(36)-C(35)-Na(2)	123.69(19)
O(1)#1-Na(2)-Na(1)	86.36(6)	O(3)-C(35)-Na(3)	44.80(12)
O(3)-Na(2)-Na(1)	87.11(6)	C(34)-C(35)-Na(3)	92.56(16)
C(35)-Na(2)-Na(1)	94.92(6)	C(36)-C(35)-Na(3)	134.03(19)
C(19)-Na(2)-Na(1)	40.48(5)	Na(2)-C(35)-Na(3)	89.04(8)
C(34)-Na(2)-Na(1)	78.16(6)	C(42)-C(36)-C(35)	118.8(3)
Na(1)#1-Na(2)-Na(1)	89.20(4)	C(42)-C(36)-C(37)	119.7(3)
Na(3)#1-Na(2)-Na(1)	47.09(3)	C(35)-C(36)-C(37)	121.4(3)
Na(3)-Na(2)-Na(1)	59.14(3)	C(39)-C(37)-C(36)	110.1(3)
O(301)-Na(3)-O(2)#1	122.15(9)	C(39)-C(37)-C(40)	111.3(3)
O(301)-Na(3)-O(3)	109.54(9)	C(36)-C(37)-C(40)	109.0(3)
O(2)#1-Na(3)-O(3)	96.27(8)	C(39)-C(37)-C(38)	106.0(3)
O(301)-Na(3)-O(1)	116.67(9)	C(36)-C(37)-C(38)	111.8(3)
O(2)#1-Na(3)-O(1)	93.49(7)	C(40)-C(37)-C(38)	108.6(3)
O(3)-Na(3)-O(1)	116.82(8)	C(41)-C(40)-C(37)	116.8(4)
O(301)-Na(3)-C(3)	92.95(9)	C(36)-C(42)-C(43)	124.1(3)
O(2)#1-Na(3)-C(3)	121.82(9)	C(49)-C(43)-C(42)	116.7(3)
O(3)-Na(3)-C(3)	115.05(8)	C(49)-C(43)-C(44)	123.7(3)