Table. Crystal data and structure refinement for benzoate **11-Bz**.

Identification code	nik15t	
Empirical formula	C25 H28 N O7.50	
Formula weight	462.48	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.7666(12) Å	α= 96.168(3)°.
	b = 11.3016(16) Å	β= 105.253(3)°.
	c = 12.5898(17) Å	γ = 106.567(2)°.
Volume	1130.8(3) $Å^3$	
Z	2	
Density (calculated)	1.358 Mg/m^3	
Absorption coefficient	0.101 mm^{-1}	
F(000)	490	
Crystal size	0.30 x 0.20 x 0.075 mm^3	
Theta range for data collection	1.71 to 28.29°.	
Index ranges	-11<=h<=10, -14<=k<=15, -11<=l<=16	
Reflections collected	7613	
Independent reflections	5290 [R(int) = 0.0541]	
Completeness to theta = 28.29°	94.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5290 / 0 / 307	
Goodness-of-fit on F2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0686, wR2 = 0.1667	
R indices (all data)	R1 = 0.1207, wR2 = 0.1986	
Largest diff. peak and hole	0.383 and -0.423 e. $Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for benzoate 11-Bz. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)

O(1)	-1084(2)	7004(2)	5306(2)	35(1)
O(2)	1420(2)	8537(2)	5926(2)	32(1)
O(3)	1958(3)	10593(2)	4405(2)	37(1)
O(4)	3809(2)	7756(2)	4515(2)	29(1)
O(5)	2079(2)	6533(2)	5306(2)	33(1)
O(6)	4593(3)	9327(2)	2106(2)	45(1)
O(7)	3861(2)	7192(2)	1892(2)	35(1)
N(1)	2166(3)	8155(2)	2323(2)	27(1)
C(1)	1067(3)	6933(2)	2331(2)	26(1)
C(2)	54(3)	6169(3)	1297(2)	32(1)
C(3)	-1041(3)	4990(3)	1241(2)	36(1)
C(4)	-1149(3)	4583(3)	2213(3)	36(1)
C(5)	-146(3)	5336(3)	3247(2)	32(1)
C(6)	997(3)	6513(2)	3322(2)	26(1)
C(7)	2101(3)	7298(2)	4482(2)	26(1)
C(8)	1521(3)	8425(2)	4802(2)	28(1)
C(9)	2710(3)	9670(2)	4774(2)	31(1)
C(10)	2799(3)	10074(2)	3722(2)	31(1)
C(11)	1717(4)	9276(3)	2592(2)	32(1)
C(12)	4437(4)	6740(3)	4728(3)	36(1)
C(13)	3531(4)	6177(4)	5517(3)	52(1)
C(14)	8(3)	7770(3)	6060(2)	30(1)
C(15)	-11(3)	8018(3)	7239(2)	32(1)
C(16)	-1482(4)	7429(3)	7464(3)	41(1)
C(17)	-1591(5)	7620(3)	8531(3)	50(1)
C(18)	-225(5)	8394(3)	9394(3)	52(1)
C(19)	1258(5)	8969(3)	9187(3)	53(1)
C(20)	1373(4)	8792(3)	8109(2)	42(1)
C(21)	3640(3)	8302(3)	2108(2)	30(1)
C(22)	5408(3)	7092(3)	1694(3)	39(1)
C(23)	5076(4)	5676(3)	1559(3)	51(1)
C(24)	5572(4)	7548(4)	627(3)	56(1)
C(25)	6915(4)	7808(4)	2707(3)	54(1)
O(8)	5428(16)	11980(12)	2345(12)	205(5)

Table 3. Bond lengths [Å] and angles [°] for benzoate 11-Bz.

O(1)-C(14)	1.199(3)
O(2)-C(14)	1.357(3)
O(2)-C(8)	1.436(3)
O(3)-C(9)	1.440(3)
O(3)-C(10)	1.448(3)
O(4)-C(7)	1.425(3)
O(4)-C(12)	1.428(3)
O(5)-C(13)	1.410(4)

O(5)-C(7)	1.420(3)
O(6)-C(21)	1.220(3)
O(7)-C(21)	1.334(3)
O(7)-C(22)	1.473(3)
N(1)-C(21)	1.357(4)
N(1)-C(1)	1.444(3)
N(1)-C(11)	1.462(4)
C(1)-C(6)	1.391(4)
C(1)-C(2)	1.393(4)
C(2)-C(3)	1.385(4)
C(3)-C(4)	1.369(4)
C(4)-C(5)	1.388(4)
C(5)-C(6)	1.395(4)
C(6)-C(7)	1.531(3)
C(7)-C(8)	1.553(4)
C(8)-C(9)	1.503(4)
C(9)-C(10)	1.461(4)
C(10)-C(11)	1.505(4)
C(12)-C(13)	1.512(4)
C(14)-C(15)	1.486(4)
C(15)-C(20)	1.388(4)
C(15)-C(16)	1.389(4)
C(16)-C(17)	1.370(4)
C(17)-C(18)	1.376(5)
C(18)-C(19)	1.382(5)
C(19)-C(20)	1.385(5)
C(22)-C(24)	1.516(5)
C(22)-C(25)	1.519(4)
C(22)-C(23)	1.525(5)

C(14)-O(2)-C(8)	116.1(2)
C(9)-O(3)-C(10)	60.74(17)
C(7)-O(4)-C(12)	105.1(2)
C(13)-O(5)-C(7)	108.5(2)
C(21)-O(7)-C(22)	121.8(2)
C(21)-N(1)-C(1)	121.9(2)
C(21)-N(1)-C(11)	118.6(2)
C(1)-N(1)-C(11)	119.5(2)
C(6)-C(1)-C(2)	120.2(2)
C(6)-C(1)-N(1)	122.3(2)
C(2)-C(1)-N(1)	117.4(2)
C(3)-C(2)-C(1)	120.6(3)
C(4)-C(3)-C(2)	119.6(3)
C(3)-C(4)-C(5)	120.3(3)
C(4)-C(5)-C(6)	121.0(3)
C(1)-C(6)-C(5)	118.2(2)

C(1)-C(6)-C(7)	122.7(2)
C(5)-C(6)-C(7)	119.1(2)
O(5)-C(7)-O(4)	104.98(19)
O(5)-C(7)-C(6)	110.3(2)
O(4)-C(7)-C(6)	110.9(2)
O(5)-C(7)-C(8)	110.0(2)
O(4)-C(7)-C(8)	109.4(2)
C(6)-C(7)-C(8)	111.1(2)
O(2)-C(8)-C(9)	105.3(2)
O(2)-C(8)-C(7)	111.8(2)
C(9)-C(8)-C(7)	112.8(2)
O(3)-C(9)-C(10)	59.91(17)
O(3)-C(9)-C(8)	116.0(2)
C(10)-C(9)-C(8)	122.2(2)
O(3)-C(10)-C(9)	59.35(17)
O(3)-C(10)-C(11)	116.5(2)
C(9)-C(10)-C(11)	122.5(2)
N(1)-C(11)-C(10)	112.6(2)
O(4)-C(12)-C(13)	102.1(2)
O(5)-C(13)-C(12)	105.4(2)
O(1)-C(14)-O(2)	123.3(3)
O(1)-C(14)-C(15)	125.2(3)
O(2)-C(14)-C(15)	111.5(2)
C(20)-C(15)-C(16)	119.6(3)
C(20)-C(15)-C(14)	122.8(3)
C(16)-C(15)-C(14)	117.6(2)
C(17)-C(16)-C(15)	120.7(3)
C(16)-C(17)-C(18)	119.8(3)
C(17)-C(18)-C(19)	120.1(3)
C(18)-C(19)-C(20)	120.4(3)
C(19)-C(20)-C(15)	119.3(3)
O(6)-C(21)-O(7)	126.2(3)
O(6)-C(21)-N(1)	122.9(3)
O(7)-C(21)-N(1)	110.8(2)
O(7)-C(22)-C(24)	109.9(3)
O(7)-C(22)-C(25)	110.4(2)
C(24)-C(22)-C(25)	112.1(3)
O(7)-C(22)-C(23)	101.1(2)
C(24)-C(22)-C(23)	111.5(3)
C(25)-C(22)-C(23)	111.2(3)

Symmetry transformations used to generate equivalent atoms:

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

	U11	U22	U33	U23	U13	U12
O(1)	34(1)	34(1)	33(1)	3(1)	8(1)	8(1)
O(2)	30(1)	36(1)	26(1)	3(1)	7(1)	8(1)
O(3)	43(1)	31(1)	42(1)	7(1)	12(1)	19(1)
O(4)	22(1)	30(1)	32(1)	7(1)	5(1)	7(1)
O(5)	34(1)	37(1)	32(1)	15(1)	11(1)	15(1)
O(6)	40(1)	34(1)	61(2)	10(1)	23(1)	3(1)
O(7)	26(1)	33(1)	48(1)	7(1)	15(1)	7(1)
N(1)	27(1)	26(1)	28(1)	8(1)	9(1)	8(1)
C(1)	21(1)	25(1)	30(1)	6(1)	6(1)	7(1)
C(2)	28(1)	37(2)	28(1)	6(1)	6(1)	11(1)
C(3)	27(1)	34(2)	38(2)	-3(1)	1(1)	8(1)
C(4)	27(1)	25(1)	51(2)	4(1)	7(1)	6(1)
C(5)	28(1)	32(2)	36(2)	12(1)	9(1)	8(1)
C(6)	22(1)	25(1)	31(1)	5(1)	5(1)	9(1)
C(7)	22(1)	28(1)	27(1)	9(1)	6(1)	4(1)
C(8)	28(1)	31(1)	21(1)	4(1)	4(1)	8(1)
C(9)	30(1)	24(1)	34(2)	2(1)	5(1)	10(1)
C(10)	28(1)	25(1)	38(2)	7(1)	7(1)	9(1)
C(11)	34(2)	28(1)	32(2)	11(1)	6(1)	11(1)
C(12)	31(2)	34(2)	44(2)	9(1)	7(1)	16(1)
C(13)	40(2)	61(2)	67(2)	39(2)	15(2)	25(2)
C(14)	33(2)	28(1)	32(2)	8(1)	9(1)	14(1)
C(15)	37(2)	33(2)	28(1)	10(1)	9(1)	16(1)
C(16)	43(2)	45(2)	36(2)	11(1)	12(1)	14(1)
C(17)	62(2)	54(2)	46(2)	21(2)	30(2)	20(2)
C(18)	80(3)	46(2)	33(2)	14(2)	24(2)	19(2)
C(19)	68(2)	44(2)	30(2)	4(1)	5(2)	5(2)
C(20)	47(2)	37(2)	34(2)	5(1)	10(1)	7(1)
C(21)	28(1)	32(2)	30(1)	6(1)	9(1)	7(1)
C(22)	26(2)	49(2)	39(2)	-1(1)	12(1)	12(1)
C(23)	38(2)	54(2)	64(2)	2(2)	15(2)	24(2)
C(24)	46(2)	70(2)	44(2)	0(2)	18(2)	6(2)
C(25)	34(2)	70(2)	49(2)	1(2)	7(1)	14(2)
O(8)	179(11)	185(12)	243(14)	75(10)	38(10)	62(9)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Figure 11-Bz.

	x	y	z	U(eq)
H(2A)	114	6455	638	38

H(3A)	-1697	4478	548	43
H(4A)	-1898	3798	2179	44
H(5A)	-238	5051	3901	38
H(8A)	416	8303	4278	33
H(9A)	3752	9994	5402	37
H(10A)	3893	10637	3742	37
H(11A)	558	9018	2581	38
H(11B)	1819	9776	2019	38
H(12A)	5639	7043	5080	43
H(12B)	4162	6135	4042	43
H(13A)	3239	5267	5369	63
H(13B)	4225	6505	6292	63
H(16A)	-2404	6899	6883	50
H(17A)	-2585	7228	8671	60
H(18A)	-299	8530	10118	62
H(19A)	2183	9478	9776	63
H(20A)	2367	9187	7970	50
H(23A)	4123	5247	913	77
H(23B)	4859	5403	2217	77
H(23C)	6037	5487	1462	77
H(24A)	5782	8441	740	84
H(24B)	4553	7130	25	84
H(24C)	6484	7362	442	84
H(25A)	7102	8696	2769	80
H(25B)	7884	7627	2617	80
H(25C)	6711	7555	3374	80
H(8C)	5179	11185	2269	307
H(8D)	6109	12387	2981	307

Table 6. Torsion angles [°] for benzoate 11-Bz.

C(21)-N(1)-C(1)-C(6)	100.7(3)
C(11)-N(1)-C(1)-C(6)	-77.2(3)
C(21)-N(1)-C(1)-C(2)	-79.5(3)
C(11)-N(1)-C(1)-C(2)	102.7(3)
C(6)-C(1)-C(2)-C(3)	0.4(4)
N(1)-C(1)-C(2)-C(3)	-179.5(3)
C(1)-C(2)-C(3)-C(4)	1.3(4)
C(2)-C(3)-C(4)-C(5)	-1.3(4)
C(3)-C(4)-C(5)-C(6)	-0.5(4)
C(2)-C(1)-C(6)-C(5)	-2.1(4)
N(1)-C(1)-C(6)-C(5)	177.8(2)
C(2)-C(1)-C(6)-C(7)	178.8(2)
N(1)-C(1)-C(6)-C(7)	-1.3(4)
C(4)-C(5)-C(6)-C(1)	2.1(4)

C(4)-C(5)-C(6)-C(7)	-178.7(3)
C(13)-O(5)-C(7)-O(4)	-20.5(3)
C(13)-O(5)-C(7)-C(6)	98.9(3)
C(13)-O(5)-C(7)-C(8)	-138.1(2)
C(12)-O(4)-C(7)-O(5)	36.1(3)
C(12)-O(4)-C(7)-C(6)	-82.9(2)
C(12)-O(4)-C(7)-C(8)	154.2(2)
C(1)-C(6)-C(7)-O(5)	-165.3(2)
C(5)-C(6)-C(7)-O(5)	15.6(3)
C(1)-C(6)-C(7)-O(4)	-49.5(3)
C(5)-C(6)-C(7)-O(4)	131.4(2)
C(1)-C(6)-C(7)-C(8)	72.4(3)
C(5)-C(6)-C(7)-C(8)	-106.7(3)
C(14)-O(2)-C(8)-C(9)	155.7(2)
C(14)-O(2)-C(8)-C(7)	-81.6(3)
O(5)-C(7)-C(8)-O(2)	10.9(3)
O(4)-C(7)-C(8)-O(2)	-104.0(2)
C(6)-C(7)-C(8)-O(2)	133.3(2)
O(5)-C(7)-C(8)-C(9)	129.2(2)
O(4)-C(7)-C(8)-C(9)	14.4(3)
C(6)-C(7)-C(8)-C(9)	-108.4(2)
C(10)-O(3)-C(9)-C(8)	-113.7(3)
O(2)-C(8)-C(9)-O(3)	-93.1(3)
C(7)-C(8)-C(9)-O(3)	144.8(2)
O(2)-C(8)-C(9)-C(10)	-162.5(2)
C(7)-C(8)-C(9)-C(10)	75.5(3)
C(9)-O(3)-C(10)-C(11)	113.7(3)
C(8)-C(9)-C(10)-O(3)	103.5(3)
O(3)-C(9)-C(10)-C(11)	-103.7(3)
C(8)-C(9)-C(10)-C(11)	-0.3(4)
C(21)-N(1)-C(11)-C(10)	-69.7(3)
C(1)-N(1)-C(11)-C(10)	108.2(3)
O(3)-C(10)-C(11)-N(1)	-138.5(2)
C(9)-C(10)-C(11)-N(1)	-69.4(3)
C(7)-O(4)-C(12)-C(13)	-36.3(3)
C(7)-O(5)-C(13)-C(12)	-2.1(3)
O(4)-C(12)-C(13)-O(5)	23.6(3)
C(8)-O(2)-C(14)-O(1)	2.6(4)
C(8)-O(2)-C(14)-C(15)	-176.5(2)
O(1)-C(14)-C(15)-C(20)	171.2(3)
O(2)-C(14)-C(15)-C(20)	-9.7(4)
O(1)-C(14)-C(15)-C(16)	-8.1(4)
O(2)-C(14)-C(15)-C(16)	171.0(2)
C(20)-C(15)-C(16)-C(17)	1.1(5)
C(14)-C(15)-C(16)-C(17)	-179.7(3)
C(15)-C(16)-C(17)-C(18)	-0.6(5)

C(16)-C(17)-C(18)-C(19)	-0.5(5)
C(17)-C(18)-C(19)-C(20)	1.2(6)
C(18)-C(19)-C(20)-C(15)	-0.8(5)
C(16)-C(15)-C(20)-C(19)	-0.4(5)
C(14)-C(15)-C(20)-C(19)	-179.6(3)
C(22)-O(7)-C(21)-O(6)	4.4(4)
C(22)-O(7)-C(21)-N(1)	-176.4(2)
C(1)-N(1)-C(21)-O(6)	-179.4(2)
C(11)-N(1)-C(21)-O(6)	-1.6(4)
C(1)-N(1)-C(21)-O(7)	1.4(3)
C(11)-N(1)-C(21)-O(7)	179.3(2)
C(21)-O(7)-C(22)-C(24)	-65.1(3)
C(21)-O(7)-C(22)-C(25)	59.2(4)
C(21)-O(7)-C(22)-C(23)	177.0(2)

Symmetry transformations used to generate equivalent atoms: