Table 1a1. Crystal data and structure refinement for 1a.

Identification code	mc4b	
Empirical formula	$C_9 H_{10} Cl N O_2$	
Formula weight	199.63	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pna21	
Unit cell dimensions	a = 11.6704(9) Å	α= 90°.
	b = 3.9682(4) Å	β= 90°.
	c = 41.889(3) Å	γ = 90°.
Volume	1939.9(3) $Å^3$	
Z	8	
Density (calculated)	1.367 Mg/m^3	
Absorption coefficient	3.232 mm^{-1}	
F(000)	832	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.11 to 70.13°.	
Index ranges	-14<=h<=12, -4<=k<=4, -48<=l<=45	
Reflections collected	10483	
Independent reflections	3390 [R(int) = 0.0781]	
Completeness to theta = 70.13°	97.7 %	
Absorption correction	Empirical	
Max. and min. transmission	0.7382 and 0.5642	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3390 / 27 / 260	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0739, wR2 = 0.1699	
R indices (all data)	R1 = 0.1201, wR2 = 0.1949	
Absolute structure parameter	0.46(6)	
Largest diff. peak and hole	0.274 and -0.294 $e.Å^{-3}$	

Table 1a2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3583(6)	-4500(20)	5943(2)	47(2)
C(2)	2903(7)	-3710(20)	5676(2)	51(2)
C(3)	3256(7)	-4470(30)	5382(2)	62(3)
C(4)	4305(8)	-6040(30)	5319(3)	66(3)
C(5)	5042(7)	-6800(30)	5580(3)	54(3)
C(6)	4657(7)	-5950(30)	5886(2)	59(2)
C(7)	3217(7)	-3900(20)	6272(2)	54(2)
C(8)	2166(9)	-3270(20)	6370(3)	51(2)
C(9)	1861(6)	-2700(20)	6718(2)	51(3)
C(10)	3934(6)	-502(19)	3640(2)	43(2)
C(11)	4628(7)	-1300(20)	3896(2)	51(2)
C(12)	4262(7)	-580(20)	4207(2)	53(2)
C(13)	3229(8)	910(30)	4268(2)	60(2)
C(14)	2599(9)	1680(30)	4013(3)	71(3)
C(15)	2891(7)	1130(20)	3705(2)	51(2)
C(16)	4304(7)	-1110(20)	3312(2)	52(2)
C(17)	5335(9)	-1760(30)	3206(3)	58(3)
C(18)	5686(6)	-2300(20)	2879(2)	57(3)
O(1)	820(6)	-2282(18)	6767(3)	69(3)
O(2)	2616(7)	-2644(19)	6929(2)	75(3)
O(3)	4932(7)	-2167(18)	2667(2)	64(2)
O(4)	6705(7)	-2930(20)	2816(3)	75(3)
Cl(1)	2396(2)	-3484(9)	5056(1)	78(1)
Cl(2)	5175(2)	-1583(9)	4526(1)	79(1)
N(1)	4313(10)	-7615(16)	7028(2)	56(3)
N(2)	3100(13)	2950(30)	2542(3)	97(4)

Table 1a3. Bond lengths [Å] and angles [°] for 1a.

C(1)-C(6)	1.399(11)
C(1)-C(2)	1.407(12)
C(1)-C(7)	1.462(12)
C(2)-C(3)	1.334(12)
C(3)-C(4)	1.398(13)
C(3)-Cl(1)	1.739(4)
C(4)-C(5)	1.423(15)
C(5)-C(6)	1.400(14)
C(7)-C(8)	1.319(13)
C(8)-C(9)	1.516(16)
C(9)-O(1)	1.243(5)
C(9)-O(2)	1.248(5)
C(10)-C(11)	1.382(11)
C(10)-C(15)	1.406(11)
C(10)-C(16)	1.457(11)
C(11)-C(12)	1.401(12)
C(12)-C(13)	1.366(12)
C(12)-Cl(2)	1.752(4)
C(13)-C(14)	1.333(16)
C(14)-C(15)	1.352(16)
C(16)-C(17)	1.308(14)
C(17)-C(18)	1.445(16)
C(18)-O(4)	1.245(5)
C(18)-O(3)	1.253(5)
C(6)-C(1)-C(2)	117.5(8)
C(6)-C(1)-C(7)	119.2(8)
C(2)-C(1)-C(7)	123.2(7)
C(3)-C(2)-C(1)	120.6(7)
C(2)-C(3)-C(4)	122.9(7)
C(2)-C(3)-Cl(1)	119.7(7)
C(4)-C(3)-Cl(1)	117.4(7)
C(3)-C(4)-C(5)	118.7(9)
C(6)-C(5)-C(4)	117.3(8)

C(5)-C(6)-C(1)	122.8(9)
C(8)-C(7)-C(1)	126.7(9)
C(7)-C(8)-C(9)	123.2(9)
O(1)-C(9)-O(2)	124.7(10)
O(1)-C(9)-C(8)	114.2(9)
O(2)-C(9)-C(8)	121.1(8)
C(11)-C(10)-C(15)	117.5(8)
C(11)-C(10)-C(16)	121.3(7)
C(15)-C(10)-C(16)	121.0(8)
C(10)-C(11)-C(12)	119.9(7)
C(13)-C(12)-C(11)	122.0(7)
C(13)-C(12)-Cl(2)	119.6(7)
C(11)-C(12)-Cl(2)	118.4(6)
C(14)-C(13)-C(12)	116.0(9)
C(13)-C(14)-C(15)	126.0(9)
C(14)-C(15)-C(10)	118.6(9)
C(17)-C(16)-C(10)	128.7(8)
C(16)-C(17)-C(18)	127.8(9)
O(4)-C(18)-O(3)	121.9(10)
O(4)-C(18)-C(17)	120.2(9)
O(3)-C(18)-C(17)	117.9(8)

Table 1a4. Anisotropic displacement parameters ($Å^2$x 10^3)for 1a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	38(4)	50(5)	51(5)	-5(4)	3(4)	-7(4)
C(2)	35(4)	61(5)	56(5)	-12(5)	-3(4)	2(4)
C(3)	42(5)	94(8)	49(5)	16(5)	-5(4)	-8(5)
C(4)	58(6)	72(7)	67(6)	3(5)	21(5)	0(5)
C(5)	26(4)	70(6)	66(6)	-2(5)	11(4)	-17(4)
C(6)	40(5)	67(7)	68(6)	-13(5)	-5(4)	1(4)
C(7)	46(5)	52(6)	64(6)	-11(5)	-5(4)	16(4)
C(8)	42(5)	47(5)	64(7)	-1(5)	-3(4)	3(4)
C(9)	49(7)	57(7)	47(7)	1(4)	-3(5)	-2(4)
C(10)	40(4)	25(4)	66(5)	-1(4)	-1(4)	-4(3)
C(11)	43(5)	55(5)	55(5)	10(5)	-2(4)	-5(4)
C(12)	61(6)	46(5)	51(5)	-7(4)	1(4)	5(4)
C(13)	53(6)	64(7)	61(6)	-16(5)	11(5)	-14(5)
C(14)	48(6)	60(6)	106(10)	-2(7)	6(6)	24(5)
C(15)	40(5)	45(5)	69(6)	4(4)	2(4)	0(4)
C(16)	40(5)	71(7)	46(5)	-1(4)	-6(4)	-11(4)
C(17)	40(5)	85(7)	48(6)	-3(6)	-11(4)	-6(5)
C(18)	41(7)	59(7)	70(9)	-17(4)	1(6)	-4(4)
O(1)	39(4)	90(6)	77(7)	-8(3)	6(4)	5(3)
O(2)	52(5)	129(9)	45(5)	-6(3)	7(4)	-1(4)
O(3)	62(5)	74(6)	55(6)	-9(3)	-15(4)	3(3)
O(4)	52(5)	106(7)	68(7)	-1(4)	9(4)	13(4)
Cl(1)	72(2)	108(2)	53(1)	2(2)	-8(1)	21(2)
Cl(2)	75(2)	101(2)	62(2)	10(2)	-10(1)	-16(2)
N(1)	83(7)	47(5)	37(6)	3(3)	4(4)	-2(3)
N(2)	107(10)	101(9)	83(10)	9(6)	15(7)	-1(6)

Table 1a5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1a.

	x	y	z	U(eq)
H(2)	2200	-2650	5705	61
H(4)	4517	-6579	5111	79
H(5)	5751	-7814	5549	64
H(6)	5137	-6357	6059	70
H(7)	3785	-3970	6428	65
H(8)	1583	-3163	6219	61
H(11)	5335	-2319	3862	61
H(13)	2980	1356	4474	72
H(14)	1893	2699	4050	86
H(15)	2413	1817	3540	62
H(16)	3730	-1035	3159	63
H(17)	5910	-1885	3359	69
H(1N)	4250(60)	-7930(160)	7245(4)	84
H(2N)	4650(50)	-9490(100)	6938(14)	84
H(3N)	4770(50)	-5760(100)	6989(16)	84
H(4N)	3600(30)	-7290(160)	6939(15)	84
H(5N)	3010(90)	2900(200)	2323(5)	146
H(6N)	2440(50)	3800(200)	2630(20)	146
H(7N)	3230(90)	820(100)	2620(20)	146
H(8N)	3710(60)	4300(200)	2590(20)	146

Table 1b1. Crystal data and structure refinement for 1b.

Identification code	mc1b	
Empirical formula	$C_9 H_{10} Br N O_2$	
Formula weight	244.09	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 42.7088(15) Å	α= 90°.
	b = 4.0066(2) Å	β= 90.411(2)°.
	c = 11.6089(6) Å	γ = 90°.
Volume	1986.43(16) $Å^3$	
Z	8	
Density (calculated)	1.632 Mg/m^3	
Absorption coefficient	5.395 mm^{-1}	
F(000)	976	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	4.14 to 70.40°.	
Index ranges	-52<=h<=44, -4<=k<=4, -13<=l<=13	
Reflections collected	5888	
Independent reflections	3113 [R(int) = 0.0405]	
Completeness to theta = 70.40°	95.6 %	
Absorption correction	Empirical	
Max. and min. transmission	0.4983 and 0.4117	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3113 / 22 / 259	
Goodness-of-fit on F^2	1.100	
Final R indices [I>2sigma(I)]	R1 = 0.0440, wR2 = 0.1112	
R indices (all data)	R1 = 0.0463, wR2 = 0.1128	
Absolute structure parameter	0.07(3)	
Largest diff. peak and hole	0.570 and -0.655 $e.Å^{-3}$	

Table 1b2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1810(2)	2022(16)	6206(5)	40(1)
C(2)	1553(2)	1164(16)	6880(6)	44(2)
C(3)	1252(2)	1827(15)	6500(6)	43(1)
C(4)	1194(2)	3407(17)	5472(6)	51(2)
C(5)	1449(2)	4290(20)	4795(6)	58(2)
C(6)	1751(2)	3585(16)	5144(6)	48(2)
C(7)	2132(2)	1453(16)	6579(6)	45(2)
C(8)	2225(2)	630(20)	7634(7)	50(2)
C(9)	2564(2)	132(16)	7969(6)	42(1)
C(10)	-548(1)	-2007(14)	3734(5)	36(1)
C(11)	-293(1)	-1232(15)	4418(5)	39(1)
C(12)	1(1)	-2048(16)	4060(5)	41(1)
C(13)	55(2)	-3543(18)	3027(6)	54(2)
C(14)	-200(2)	-4318(19)	2335(6)	53(2)
C(15)	-500(2)	-3576(18)	2674(6)	49(2)
C(16)	-872(2)	-1335(16)	4100(6)	45(2)
C(17)	-970(2)	-828(17)	5157(6)	43(2)
C(18)	-1299(2)	-129(16)	5505(6)	44(2)
O(1)	2770(1)	386(15)	7204(4)	61(2)
O(2)	2617(1)	-443(14)	8998(4)	62(1)
O(3)	-1509(1)	-138(15)	4728(4)	58(1)
O(4)	-1352(1)	291(15)	6547(4)	62(1)
Br(1)	913(1)	529(3)	7456(1)	67(1)
Br(2)	349(1)	-941(2)	5028(1)	61(1)
N(1)	2880(2)	5446(17)	5440(7)	66(2)
N(2)	-1613(2)	5110(18)	7983(7)	70(2)

Table 1b3. Bond lengths [Å] and angles [°] for 1b.

C(1)-C(2)	1.395(9)
C(1)-C(6)	1.404(9)
C(1)-C(7)	1.458(9)
C(2)-C(3)	1.383(9)
C(3)-C(4)	1.372(10)
C(3)-Br(1)	1.901(7)
C(4)-C(5)	1.392(12)
C(5)-C(6)	1.377(11)
C(7)-C(8)	1.325(10)
C(8)-C(9)	1.510(10)
C(9)-O(2)	1.237(8)
C(9)-O(1)	1.259(8)
C(10)-C(11)	1.379(8)
C(10)-C(15)	1.398(9)
C(10)-C(16)	1.474(9)
C(11)-C(12)	1.367(8)
C(12)-C(13)	1.362(9)
C(12)-Br(2)	1.910(6)
C(13)-C(14)	1.382(11)
C(14)-C(15)	1.375(11)
C(16)-C(17)	1.315(10)
C(17)-C(18)	1.490(10)
C(18)-O(4)	1.244(8)
C(18)-O(3)	1.267(8)
C(2)-C(1)-C(6)	117.8(6)
C(2)-C(1)-C(7)	122.6(6)
C(6)-C(1)-C(7)	119.6(6)
C(3)-C(2)-C(1)	120.5(6)
C(4)-C(3)-C(2)	121.8(6)
C(4)-C(3)-Br(1)	120.2(5)
C(2)-C(3)-Br(1)	118.1(5)
C(3)-C(4)-C(5)	118.2(7)
C(6)-C(5)-C(4)	121.1(7)

C(5)-C(6)-C(1)	120.7(7)
C(8)-C(7)-C(1)	126.0(6)
C(7)-C(8)-C(9)	123.3(7)
O(2)-C(9)-O(1)	124.9(6)
O(2)-C(9)-C(8)	116.3(6)
O(1)-C(9)-C(8)	118.8(6)
C(11)-C(10)-C(15)	119.1(6)
C(11)-C(10)-C(16)	122.1(5)
C(15)-C(10)-C(16)	118.7(6)
C(12)-C(11)-C(10)	119.7(6)
C(13)-C(12)-C(11)	122.2(6)
C(13)-C(12)-Br(2)	119.1(5)
C(11)-C(12)-Br(2)	118.7(5)
C(12)-C(13)-C(14)	118.3(7)
C(15)-C(14)-C(13)	121.0(7)
C(14)-C(15)-C(10)	119.6(7)
C(17)-C(16)-C(10)	127.1(6)
C(16)-C(17)-C(18)	126.1(7)
O(4)-C(18)-O(3)	124.0(6)
O(4)-C(18)-C(17)	117.9(6)
O(3)-C(18)-C(17)	118.0(6)

Table 1b4. Anisotropic displacement parameters ($Å^2$x 10^3)for 1b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	44(3)	41(3)	36(3)	-6(3)	-4(3)	3(2)
C(2)	47(4)	42(4)	42(3)	-1(3)	-2(3)	1(3)
C(3)	47(4)	34(3)	48(4)	-6(3)	-1(3)	0(2)
C(4)	47(4)	51(4)	56(4)	-3(3)	-8(3)	10(3)
C(5)	66(5)	70(5)	38(4)	0(4)	-10(3)	4(4)
C(6)	53(4)	48(4)	43(3)	-2(3)	9(3)	3(3)
C(7)	50(4)	44(4)	41(3)	4(3)	11(3)	1(3)
C(8)	32(4)	77(5)	41(4)	1(3)	3(3)	5(3)
C(9)	40(4)	46(4)	41(4)	1(3)	0(3)	-1(3)
C(10)	40(3)	30(3)	36(3)	7(2)	3(3)	-3(2)
C(11)	36(3)	46(3)	34(3)	-6(3)	-1(3)	3(2)
C(12)	34(3)	49(4)	40(3)	0(3)	-1(3)	0(2)
C(13)	48(4)	58(4)	55(4)	-2(3)	14(3)	-1(3)
C(14)	58(4)	59(5)	41(4)	-4(3)	8(3)	-3(3)
C(15)	53(4)	57(5)	37(3)	-1(3)	-1(3)	1(3)
C(16)	40(3)	52(4)	42(4)	1(3)	-9(3)	-1(3)
C(17)	35(4)	53(4)	41(4)	2(3)	2(3)	7(3)
C(18)	37(4)	47(4)	47(4)	5(3)	1(3)	0(3)
O(1)	40(3)	102(4)	42(3)	-2(3)	1(2)	8(3)
O(2)	56(3)	88(4)	41(3)	6(3)	-5(2)	10(3)
O(3)	36(3)	93(4)	44(3)	-6(3)	-7(2)	9(2)
O(4)	50(3)	94(4)	43(3)	-7(3)	8(2)	6(3)
Br(1)	38(1)	93(1)	72(1)	-1(1)	5(1)	-3(1)
Br(2)	35(1)	70(1)	77(1)	-9(1)	-4(1)	-6(1)
N(1)	39(3)	56(4)	103(5)	-9(4)	-8(4)	6(3)
N(2)	39(3)	65(4)	106(6)	1(4)	8(4)	10(3)

Table 1b5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1b.

	x	y	z	U(eq)
H(2)	1585	140	7590	52
H(4)	991	3876	5233	62
H(5)	1415	5372	4097	70
H(6)	1917	4151	4670	58
H(7)	2287	1688	6026	54
H(8)	2073	349	8196	59
H(11)	-322	-159	5120	46
H(13)	257	-4030	2792	64
H(14)	-168	-5358	1629	63
H(15)	-669	-4114	2202	59
H(16)	-1024	-1261	3521	53
H(17)	-821	-915	5742	51
H(1N)	2855(16)	7120(120)	5980(40)	99
H(2N)	2806(15)	3480(90)	5730(50)	99
H(3N)	3090(5)	5270(170)	5270(60)	99
H(4N)	2770(15)	6030(160)	4780(40)	99
H(5N)	-1484(14)	5110(170)	7350(40)	105
H(6N)	-1534(15)	6550(140)	8530(40)	105
H(7N)	-1619(17)	2980(70)	8290(60)	105
H(8N)	-1811(7)	5760(170)	7770(60)	105

Table 2a1. Crystal data and structure refinement for 2a.

Identification code	mc4	
Empirical formula	C18 H17 Cl2 N O4	
Formula weight	382.23	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 39.987(2) Å	α= 90°.
	b = 5.9313(3) Å	β= 94.379(4)°.
	c = 7.5657(4) Å	γ = 90°.
Volume	1789.14(16) $Å^3$	
Z	4	
Density (calculated)	1.419 Mg/m^3	
Absorption coefficient	3.465 mm^{-1}	
F(000)	792	
Crystal size	0.30 x 0.20 x 0.08 mm^3	
Theta range for data collection	4.44 to 70.50°.	
Index ranges	-46<=h<=45, -7<=k<=6, -9<=l<=9	
Reflections collected	5248	
Independent reflections	1592 [R(int) = 0.0580]	
Completeness to theta = 70.50°	92.8 %	
Absorption correction	Empirical	
Max. and min. transmission	0.7690 and 0.4229	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1592 / 2 / 122	
Goodness-of-fit on F^2	1.077	
Final R indices [I>2sigma(I)]	R1 = 0.0763, wR2 = 0.1971	
R indices (all data)	R1 = 0.0849, wR2 = 0.2054	
Largest diff. peak and hole	0.772 and -0.427 e.$Å^{-3}$	

Table 2a2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3693(1)	2053(8)	2336(5)	56(1)
C(2)	3418(1)	626(7)	2471(5)	53(1)
C(3)	3105(1)	1293(7)	1782(5)	48(1)
C(4)	3058(1)	3352(7)	950(5)	53(1)
C(5)	3332(1)	4734(8)	814(6)	59(1)
C(6)	3645(1)	4115(8)	1490(6)	60(1)
C(7)	4039(1)	1507(10)	3056(6)	68(1)
C(8)	4141(1)	-435(9)	3592(6)	72(1)
C(9)	4497(1)	-1011(11)	4279(7)	71(1)
N(1)	5000	4639(13)	2500	72(2)
O(1)	4705(1)	666(8)	4477(7)	103(2)
O(2)	4564(1)	-2904(7)	4610(5)	81(1)
Cl(1)	2763(1)	-497(2)	1900(2)	70(1)

Table 2a3. Bond lengths [Å] and angles [°] for 2a.

C(1)-C(6)	1.387(7)
C(1)-C(2)	1.398(6)
C(1)-C(7)	1.483(6)
C(2)-C(3)	1.377(6)
C(3)-C(4)	1.380(6)
C(3)-Cl(1)	1.739(4)
C(4)-C(5)	1.379(6)
C(5)-C(6)	1.366(6)
C(7)-C(8)	1.278(7)
C(8)-C(9)	1.517(7)
C(9)-O(2)	1.177(7)
C(9)-O(1)	1.298(7)
C(6)-C(1)-C(2)	119.1(4)
C(6)-C(1)-C(7)	117.0(4)
C(2)-C(1)-C(7)	123.9(4)
C(3)-C(2)-C(1)	119.7(4)
C(2)-C(3)-C(4)	121.0(4)
C(2)-C(3)-Cl(1)	120.0(3)
C(4)-C(3)-Cl(1)	119.0(3)
C(5)-C(4)-C(3)	118.6(4)
C(6)-C(5)-C(4)	121.5(4)
C(5)-C(6)-C(1)	120.0(4)
C(8)-C(7)-C(1)	125.5(6)
C(7)-C(8)-C(9)	125.5(6)
O(2)-C(9)-O(1)	124.9(5)
O(2)-C(9)-C(8)	118.7(6)
O(1)-C(9)-C(8)	116.3(5)

Table 2a4. Anisotropic displacement parameters ($Å^2$x 10^3)for 2a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	47(2)	78(3)	42(2)	-8(2)	5(2)	8(2)
C(2)	60(3)	57(2)	42(2)	2(2)	5(2)	17(2)
C(3)	49(2)	52(2)	42(2)	-2(2)	4(2)	7(2)
C(4)	50(2)	60(2)	47(2)	0(2)	-2(2)	15(2)
C(5)	68(3)	59(3)	51(2)	-1(2)	5(2)	7(2)
C(6)	60(3)	66(3)	53(2)	-4(2)	9(2)	-2(2)
C(7)	65(3)	82(3)	59(3)	4(2)	10(2)	11(3)
C(8)	78(3)	75(3)	63(3)	0(2)	12(2)	-1(3)
C(9)	59(3)	98(4)	59(3)	17(3)	18(2)	9(3)
N(1)	84(5)	82(5)	51(3)	0	11(3)	0
O(1)	76(3)	99(3)	137(4)	54(3)	15(3)	33(2)
O(2)	68(2)	98(3)	76(2)	17(2)	8(2)	25(2)
Cl(1)	57(1)	75(1)	76(1)	13(1)	-1(1)	-5(1)

Table 2a5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2a.

	x	y	z	U(eq)
H(2)	3446	-769	3024	64
H(4)	2846	3798	490	63
H(5)	3303	6121	249	71
H(6)	3826	5076	1383	71
H(7)	4194	2676	3124	82
H(8)	3984	-1594	3557	86
H(10)	5147(15)	5430(110)	1910(90)	130(30)
H(1)	5000	0	5000	105
H(9)	4868(17)	3730(100)	1790(90)	140(30)

Table 2b1. Crystal data and structure refinement for 2b.

Identification code	mc1	
Empirical formula	$C_{18} H_{17} Br_2 N O_4$	
Formula weight	471.15	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12$	
Unit cell dimensions	a = 5.5664(3) Å	α= 90°.
	b = 40.672(2) Å	β= 90°.
	c = 3.9542(3) Å	γ = 90°.
Volume	895.21(10) $Å^3$	
Z	2	
Density (calculated)	1.748 Mg/m^3	
Absorption coefficient	5.947 mm^{-1}	
F(000)	468	
Crystal size	0.30 x 0.30 x 0.10 mm^3	
Theta range for data collection	2.17 to 70.26°.	
Index ranges	-6<=h<=6, -49<=k<=48, -4<=l<=4	
Reflections collected	5394	
Independent reflections	1561 [R(int) = 0.0476]	
Completeness to theta = 70.26°	96.1 %	
Absorption correction	Empirical	
Max. and min. transmission	0.5877 and 0.1026	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1561 / 0 / 124	
Goodness-of-fit on F^2	1.341	
Final R indices [I>2sigma(I)]	R1 = 0.0404, wR2 = 0.0971	
R indices (all data)	R1 = 0.0409, wR2 = 0.0973	
Absolute structure parameter	0.03(5)	
Largest diff. peak and hole	0.425 and -0.706 $e.Å^{-3}$	

Table 2b2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6750(8)	6260(1)	7834(13)	29(1)
C(2)	8050(9)	6536(1)	6828(14)	33(1)
C(3)	7215(9)	6846(1)	7601(14)	31(1)
C(4)	5106(9)	6896(1)	9263(15)	39(1)
C(5)	3806(10)	6622(1)	10280(15)	42(1)
C(6)	4610(9)	6307(1)	9567(13)	35(1)
C(7)	7575(9)	5924(1)	7040(13)	32(1)
C(8)	9615(9)	5844(1)	5580(15)	35(1)
C(9)	10449(9)	5506(1)	4892(15)	36(1)
N(1)	5000	5000	9880(20)	39(2)
O(1)	8987(7)	5270(1)	5574(11)	46(1)
O(2)	12502(7)	5464(1)	3826(16)	57(1)
Br(1)	9054(1)	7216(1)	6144(2)	46(1)

Table 2b3. Bond lengths [Å] and angles [°] for 2b.

C(1)-C(6)	1.387(7)
C(1)-C(2)	1.393(7)
C(1)-C(7)	1.475(6)
C(2)-C(3)	1.377(6)
C(3)-C(4)	1.361(8)
C(3)-Br(1)	1.909(5)
C(4)-C(5)	1.390(8)
C(5)-C(6)	1.385(7)
C(7)-C(8)	1.315(7)
C(8)-C(9)	1.476(7)
C(9)-O(2)	1.230(6)
C(9)-O(1)	1.287(6)
C(6)-C(1)-C(2)	118.4(5)
C(6)-C(1)-C(7)	120.0(4)
C(2)-C(1)-C(7)	121.6(4)
C(3)-C(2)-C(1)	119.9(5)
C(4)-C(3)-C(2)	122.5(5)
C(4)-C(3)-Br(1)	119.3(4)
C(2)-C(3)-Br(1)	118.2(4)
C(3)-C(4)-C(5)	117.8(5)
C(6)-C(5)-C(4)	121.0(5)
C(5)-C(6)-C(1)	120.3(5)
C(8)-C(7)-C(1)	126.3(5)
C(7)-C(8)-C(9)	125.7(5)
O(2)-C(9)-O(1)	123.7(5)
O(2)-C(9)-C(8)	119.0(5)
O(1)-C(9)-C(8)	117.2(4)

Table 2b4. Anisotropic displacement parameters ($Å^2$x 10^3)for 2b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	29(2)	25(2)	32(3)	0(2)	-4(2)	0(2)
C(2)	27(2)	29(2)	43(3)	-1(2)	1(2)	4(2)
C(3)	34(3)	25(2)	33(3)	-3(2)	-3(2)	2(2)
C(4)	41(3)	33(3)	42(3)	-12(3)	-4(3)	7(2)
C(5)	31(2)	46(3)	50(3)	-9(3)	5(3)	6(2)
C(6)	34(3)	39(3)	32(3)	0(2)	4(2)	-3(2)
C(7)	30(2)	23(2)	43(3)	3(2)	3(2)	-3(2)
C(8)	34(3)	24(2)	46(3)	0(2)	10(2)	-2(2)
C(9)	32(3)	30(3)	47(3)	-6(2)	1(2)	4(2)
N(1)	37(3)	37(4)	43(4)	0	0	3(3)
O(1)	39(2)	24(2)	74(3)	1(2)	10(2)	4(2)
O(2)	39(2)	36(2)	96(3)	-15(3)	21(3)	2(2)
Br(1)	60(1)	25(1)	54(1)	3(1)	-1(1)	-4(1)

Table 2b5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2b.

	x	y	z	U(eq)
H(2)	9480	6511	5638	40
H(4)	4553	7108	9705	46
H(5)	2374	6650	11457	51
H(6)	3711	6126	10255	42
H(7)	6554	5752	7629	38
H(8)	10620	6015	4925	42
H(1)	10000	5000	5400(400)	130(50)
H(9)	4290(130)	5157(16)	11200(200)	70(20)
H(10)	3880(120)	4892(16)	8660(190)	60(20)