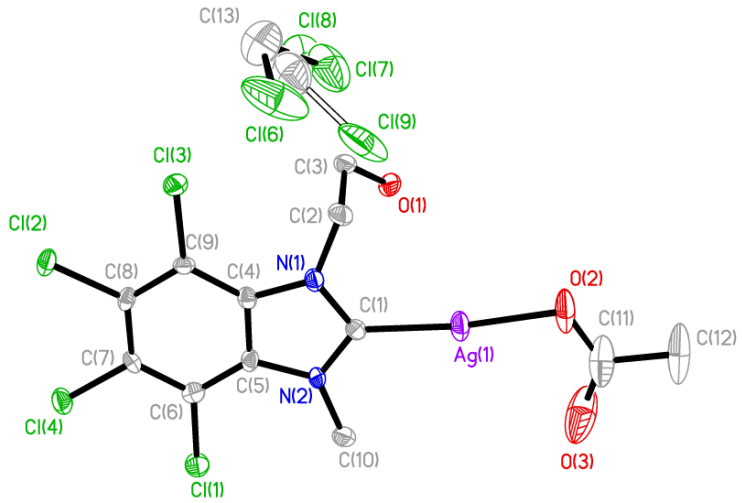

Asymmetric unit of $C_{12}H_{11}N_2O_3Cl_4Ag_1$ containing one disordered molecule of $C_1H_2Cl_2$ with thermal ellipsoids drawn at 50% probability.

Table 1. Crystal data and structure refinement for bw.

Identification code	bw	
Empirical formula	C13 H13 Ag Cl6 N2 O3	
Formula weight	565.82	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 8.616(3) Å	α= 90°.
	b = 13.028(5) Å	β= 92.684(5)°.
	c = 17.176(6) Å	γ = 90°.
Volume	1925.9(12) $Å^3$	
Z	4	
Density (calculated)	1.951 Mg/m^3	
Absorption coefficient	1.895 mm^{-1}	
F(000)	1112	
Crystal size	0.27 x 0.10 x 0.04 mm^3	

Theta range for data collection	1.96 to 26.30°.
Index ranges	-10<=h<=10, -16<=k<=16, -21<=l<=21
Reflections collected	14692
Independent reflections	3909 [R(int) = 0.0908]
Completeness to theta = 26.30°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9213 and 0.6327
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3909 / 0 / 257
Goodness-of-fit on F^2	1.015
Final R indices [I>2sigma(I)]	R1 = 0.0528, wR2 = 0.1296
R indices (all data)	R1 = 0.0655, wR2 = 0.1389
Largest diff. peak and hole	1.593 and -0.836 e.Å^{-3}

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

	x	y	z	U(eq)
Ag(1)	3214(1)	4598(1)	9942(1)	28(1)
Cl(1)	7785(1)	1457(1)	11630(1)	27(1)
Cl(2)	7455(1)	-932(1)	9070(1)	24(1)
Cl(3)	5203(1)	589(1)	8209(1)	24(1)
Cl(4)	8668(1)	-519(1)	10766(1)	26(1)
Cl(6)	-996(3)	227(3)	7316(2)	78(1)
Cl(7)	1256(6)	1839(4)	6990(3)	70(1)
Cl(8)	1867(7)	1617(5)	6827(4)	47(1)
Cl(9)	-828(4)	1538(4)	7766(2)	69(2)
O(1)	5317(4)	4291(2)	8317(2)	28(1)
O(2)	1669(4)	5838(3)	9776(3)	48(1)
O(3)	1975(6)	6198(4)	11015(4)	85(2)
N(1)	4495(4)	2575(3)	9351(2)	19(1)
N(2)	5377(4)	2850(3)	10541(2)	18(1)
C(1)	4468(5)	3240(3)	9958(2)	19(1)
C(2)	3718(5)	2801(3)	8594(2)	24(1)
C(3)	4798(6)	3318(3)	8041(2)	25(1)
C(4)	5467(5)	1748(3)	9549(2)	17(1)
C(5)	6033(5)	1922(3)	10309(2)	18(1)
C(6)	7030(5)	1238(3)	10700(2)	19(1)
C(7)	7458(5)	363(3)	10301(3)	17(1)
C(8)	6893(5)	176(3)	9529(2)	17(1)
C(9)	5896(5)	864(3)	9143(2)	18(1)
C(10)	5626(6)	3360(3)	11293(3)	27(1)
C(11)	1369(6)	6335(4)	10371(5)	51(2)
C(12)	189(7)	7191(4)	10281(5)	68(2)
C(13)	520(17)	577(10)	6749(9)	51(3)
C(14)	270(20)	922(14)	7065(12)	49(5)

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

Ag(1)-C(1)	2.072(4)
Ag(1)-O(2)	2.104(4)
Ag(1)-Ag(1)#1	3.2494(13)
Cl(1)-C(6)	1.720(4)
Cl(2)-C(8)	1.725(4)
Cl(3)-C(9)	1.723(4)
Cl(4)-C(7)	1.723(4)
Cl(6)-C(13)	1.728(15)
Cl(7)-C(13)	1.803(14)
Cl(8)-C(14)	1.71(2)
Cl(9)-C(14)	1.76(2)
O(1)-C(3)	1.418(5)
O(1)-H(1)	0.8200
O(2)-C(11)	1.248(8)
O(3)-C(11)	1.214(8)
N(1)-C(1)	1.357(5)
N(1)-C(4)	1.397(5)
N(1)-C(2)	1.464(5)
N(2)-C(1)	1.342(5)
N(2)-C(5)	1.401(5)
N(2)-C(10)	1.460(5)
C(2)-C(3)	1.518(6)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.390(6)
C(4)-C(9)	1.404(6)
C(5)-C(6)	1.389(6)
C(6)-C(7)	1.389(6)
C(7)-C(8)	1.412(6)
C(8)-C(9)	1.388(6)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600

C(10)-H(10C)	0.9600
C(11)-C(12)	1.512(7)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700

C(1)-Ag(1)-O(2)	169.53(17)
C(1)-Ag(1)-Ag(1)#1	77.45(12)
O(2)-Ag(1)-Ag(1)#1	110.59(11)
C(3)-O(1)-H(1)	109.5
C(11)-O(2)-Ag(1)	116.2(4)
C(1)-N(1)-C(4)	109.7(3)
C(1)-N(1)-C(2)	122.0(4)
C(4)-N(1)-C(2)	128.0(4)
C(1)-N(2)-C(5)	110.1(3)
C(1)-N(2)-C(10)	123.0(4)
C(5)-N(2)-C(10)	126.9(4)
N(2)-C(1)-N(1)	107.5(4)
N(2)-C(1)-Ag(1)	128.2(3)
N(1)-C(1)-Ag(1)	124.2(3)
N(1)-C(2)-C(3)	112.1(4)
N(1)-C(2)-H(2A)	109.2
C(3)-C(2)-H(2A)	109.2
N(1)-C(2)-H(2B)	109.2
C(3)-C(2)-H(2B)	109.2
H(2A)-C(2)-H(2B)	107.9
O(1)-C(3)-C(2)	112.4(4)
O(1)-C(3)-H(3A)	109.1
C(2)-C(3)-H(3A)	109.1
O(1)-C(3)-H(3B)	109.1
C(2)-C(3)-H(3B)	109.1
H(3A)-C(3)-H(3B)	107.9

C(5)-C(4)-N(1)	106.4(3)
C(5)-C(4)-C(9)	120.7(4)
N(1)-C(4)-C(9)	132.9(4)
C(6)-C(5)-C(4)	122.1(4)
C(6)-C(5)-N(2)	131.6(4)
C(4)-C(5)-N(2)	106.3(4)
C(7)-C(6)-C(5)	117.4(4)
C(7)-C(6)-Cl(1)	119.8(3)
C(5)-C(6)-Cl(1)	122.8(3)
C(6)-C(7)-C(8)	121.2(4)
C(6)-C(7)-Cl(4)	119.1(3)
C(8)-C(7)-Cl(4)	119.7(3)
C(9)-C(8)-C(7)	121.0(4)
C(9)-C(8)-Cl(2)	120.2(3)
C(7)-C(8)-Cl(2)	118.8(3)
C(8)-C(9)-C(4)	117.7(4)
C(8)-C(9)-Cl(3)	119.3(3)
C(4)-C(9)-Cl(3)	123.0(3)
N(2)-C(10)-H(10A)	109.5
N(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
N(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
O(3)-C(11)-O(2)	125.0(5)
O(3)-C(11)-C(12)	117.4(7)
O(2)-C(11)-C(12)	117.6(7)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Cl(6)-C(13)-Cl(7)	112.2(8)
Cl(6)-C(13)-H(13A)	109.2
Cl(7)-C(13)-H(13A)	109.2

Cl(6)-C(13)-H(13B)	109.2
Cl(7)-C(13)-H(13B)	109.2
H(13A)-C(13)-H(13B)	107.9
Cl(8)-C(14)-Cl(9)	112.7(11)
Cl(8)-C(14)-H(14A)	109.1
Cl(9)-C(14)-H(14A)	109.1
Cl(8)-C(14)-H(14B)	109.1
Cl(9)-C(14)-H(14B)	109.1
H(14A)-C(14)-H(14B)	107.8

Symmetry transformations used to generate equivalent atoms:

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

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	30(1)	16(1)	38(1)	4(1)	6(1)	6(1)
Cl(1)	34(1)	25(1)	22(1)	-4(1)	-8(1)	2(1)
Cl(2)	29(1)	16(1)	29(1)	-5(1)	4(1)	3(1)
Cl(3)	32(1)	20(1)	18(1)	-3(1)	-1(1)	-1(1)
Cl(4)	26(1)	21(1)	30(1)	3(1)	-2(1)	7(1)
Cl(6)	35(2)	141(4)	57(2)	48(2)	-3(1)	-5(2)
Cl(7)	77(3)	48(2)	80(3)	4(2)	-41(3)	-3(2)
Cl(8)	38(3)	53(3)	49(2)	-1(2)	2(2)	-4(2)
Cl(9)	40(2)	120(4)	47(2)	49(3)	12(2)	35(2)
O(1)	50(2)	12(2)	23(2)	0(1)	8(2)	0(1)
O(2)	39(2)	24(2)	83(3)	12(2)	18(2)	15(2)
O(3)	56(3)	82(4)	114(4)	-63(3)	-36(3)	29(3)
N(1)	20(2)	15(2)	21(2)	3(1)	3(1)	2(1)
N(2)	27(2)	10(2)	19(2)	2(1)	4(2)	2(1)
C(1)	24(2)	15(2)	18(2)	3(2)	4(2)	0(2)
C(2)	27(2)	24(2)	19(2)	0(2)	-8(2)	2(2)
C(3)	45(3)	15(2)	15(2)	0(2)	-2(2)	1(2)
C(4)	17(2)	13(2)	21(2)	2(2)	2(2)	-2(2)
C(5)	22(2)	10(2)	22(2)	0(2)	5(2)	-1(2)
C(6)	19(2)	20(2)	19(2)	-1(2)	2(2)	-3(2)
C(7)	18(2)	14(2)	19(2)	5(2)	0(2)	1(2)
C(8)	15(2)	13(2)	24(2)	-1(2)	8(2)	0(2)
C(9)	22(2)	18(2)	12(2)	0(2)	0(2)	-1(2)
C(10)	45(3)	20(2)	18(2)	2(2)	3(2)	2(2)
C(11)	24(3)	21(3)	107(6)	-12(3)	-3(3)	-4(2)
C(12)	30(3)	25(3)	150(7)	-3(4)	12(4)	8(2)
C(13)	48(7)	44(8)	62(9)	-9(6)	5(7)	-11(6)
C(14)	54(12)	35(11)	58(13)	5(9)	-9(10)	-8(8)

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

	x	y	z	U(eq)
H(1)	4832	4454	8697	42
H(2A)	2834	3245	8671	28
H(2B)	3332	2167	8361	28
H(3A)	5692	2879	7973	30
H(3B)	4260	3402	7537	30
H(10A)	5051	3992	11292	41
H(10B)	6713	3503	11384	41
H(10C)	5278	2921	11699	41
H(12A)	103	7535	10771	102
H(12B)	-802	6910	10116	102
H(12C)	517	7672	9898	102
H(13A)	167	565	6204	61
H(13B)	1354	81	6820	61
H(14A)	608	257	7265	59
H(14B)	-383	806	6598	59

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