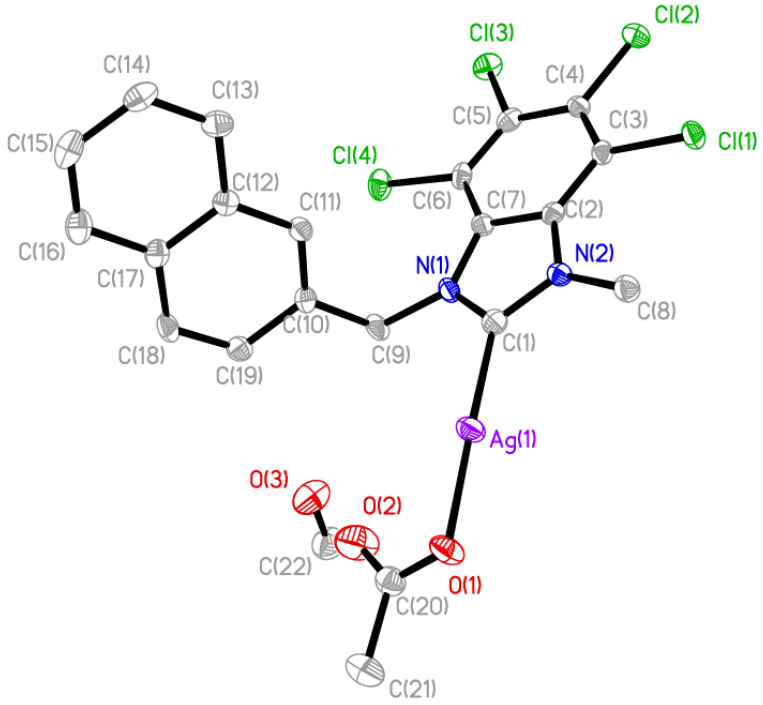

Asymmetric unit of $C_{21}H_{15}N_2O_2Cl_4Ag_1$ containing one molecule of $C_1H_4O_1$ with thermal ellipsoids drawn at 50% probability.

Table 1. Crystal data and structure refinement for bw.

Identification code	bw	
Empirical formula	C22 H19 Ag Cl4 N2 O3	
Formula weight	609.06	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.1480(4) Å	α= 106.8060(10)°.
	b = 11.5407(4) Å	β= 105.3150(10)°.
	c = 12.1076(5) Å	γ = 111.7690(10)°.
Volume	1145.37(8) $Å^3$	
Z	2	
Density (calculated)	1.766 Mg/m^3	
Absorption coefficient	11.596 mm^{-1}	

F(000)	608
Crystal size	0.15 x 0.06 x 0.04 mm^3
Theta range for data collection	4.20 to 66.36°.
Index ranges	-12<=h<=12, -13<=k<=13, -10<=l<=13
Reflections collected	7216
Independent reflections	3486 [R(int) = 0.0227]
Completeness to theta = 66.36°	86.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6294 and 0.2751
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3486 / 0 / 293
Goodness-of-fit on F^2	1.323
Final R indices [I>2sigma(I)]	R1 = 0.0239, wR2 = 0.0662
R indices (all data)	R1 = 0.0243, wR2 = 0.0667
Largest diff. peak and hole	0.542 and -0.431 $e.Å^{-3}$

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)	-157(1)	-475(1)	3542(1)	22(1)
Cl(1)	4511(1)	-1751(1)	6881(1)	21(1)
Cl(2)	8018(1)	455(1)	8337(1)	23(1)
Cl(3)	9190(1)	3301(1)	8247(1)	25(1)
Cl(4)	6887(1)	4069(1)	6801(1)	26(1)
O(1)	-2383(2)	-1117(2)	2156(2)	27(1)
O(2)	-982(2)	817(2)	2067(2)	44(1)
O(3)	1698(2)	2783(2)	2189(2)	39(1)
N(1)	3340(2)	1373(2)	5254(2)	18(1)
N(2)	2525(2)	-618(2)	5324(2)	17(1)
C(1)	2057(2)	135(2)	4811(2)	18(1)
C(2)	4117(2)	137(2)	6099(2)	16(1)
C(3)	5139(2)	-178(2)	6810(2)	16(1)
C(4)	6709(2)	814(2)	7471(2)	17(1)
C(5)	7236(2)	2113(2)	7429(2)	19(1)
C(6)	6215(3)	2438(2)	6750(2)	19(1)
C(7)	4636(2)	1422(2)	6059(2)	17(1)
C(8)	1427(2)	-2015(2)	5093(2)	20(1)
C(9)	3232(3)	2440(2)	4856(2)	21(1)
C(10)	2877(2)	3406(2)	5716(2)	18(1)
C(11)	3120(2)	3590(2)	6932(2)	18(1)
C(12)	2806(2)	4548(2)	7712(2)	18(1)
C(13)	3075(2)	4765(2)	8982(2)	23(1)
C(14)	2787(3)	5703(2)	9709(2)	26(1)
C(15)	2191(3)	6461(2)	9205(3)	28(1)
C(16)	1895(3)	6256(2)	7981(2)	25(1)
C(17)	2203(2)	5303(2)	7199(2)	19(1)
C(18)	1927(2)	5060(2)	5924(2)	20(1)
C(19)	2267(3)	4152(2)	5202(2)	20(1)
C(20)	-2229(3)	-249(2)	1686(2)	24(1)
C(21)	-3666(3)	-542(3)	649(3)	33(1)

C(22)	1909(4)	2606(3)	1073(3)	38(1)

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

Ag(1)-C(1)	2.069(2)
Ag(1)-O(1)	2.1223(16)
Ag(1)-Ag(1)#1	3.2663(3)
Cl(1)-C(3)	1.723(2)
Cl(2)-C(4)	1.720(2)
Cl(3)-C(5)	1.718(2)
Cl(4)-C(6)	1.724(2)
O(1)-C(20)	1.270(3)
O(2)-C(20)	1.239(3)
O(3)-C(22)	1.393(4)
N(1)-C(1)	1.354(3)
N(1)-C(7)	1.385(3)
N(1)-C(9)	1.475(3)
N(2)-C(1)	1.353(3)
N(2)-C(2)	1.390(3)
N(2)-C(8)	1.470(3)
C(2)-C(3)	1.392(3)
C(2)-C(7)	1.398(3)
C(3)-C(4)	1.391(3)
C(4)-C(5)	1.414(3)
C(5)-C(6)	1.381(3)
C(6)-C(7)	1.405(3)
C(9)-C(10)	1.510(3)
C(10)-C(11)	1.364(4)
C(10)-C(19)	1.420(3)
C(11)-C(12)	1.425(3)
C(12)-C(13)	1.416(4)
C(12)-C(17)	1.423(3)
C(13)-C(14)	1.361(3)
C(14)-C(15)	1.418(4)
C(15)-C(16)	1.361(4)
C(16)-C(17)	1.418(3)
C(17)-C(18)	1.416(4)
C(18)-C(19)	1.371(3)

C(20)-C(21)	1.497(4)
C(1)-Ag(1)-O(1)	176.68(7)
C(1)-Ag(1)-Ag(1)#1	68.45(6)
O(1)-Ag(1)-Ag(1)#1	114.86(5)
C(20)-O(1)-Ag(1)	108.08(14)
C(1)-N(1)-C(7)	110.57(18)
C(1)-N(1)-C(9)	120.42(19)
C(7)-N(1)-C(9)	129.01(19)
C(1)-N(2)-C(2)	110.44(18)
C(1)-N(2)-C(8)	122.20(18)
C(2)-N(2)-C(8)	127.32(19)
N(2)-C(1)-N(1)	106.65(18)
N(2)-C(1)-Ag(1)	127.60(16)
N(1)-C(1)-Ag(1)	125.71(16)
C(3)-C(2)-N(2)	132.4(2)
C(3)-C(2)-C(7)	121.44(19)
N(2)-C(2)-C(7)	106.11(19)
C(4)-C(3)-C(2)	118.3(2)
C(4)-C(3)-Cl(1)	119.82(17)
C(2)-C(3)-Cl(1)	121.91(16)
C(3)-C(4)-C(5)	120.3(2)
C(3)-C(4)-Cl(2)	119.80(17)
C(5)-C(4)-Cl(2)	119.85(16)
C(6)-C(5)-C(4)	121.31(19)
C(6)-C(5)-Cl(3)	119.94(17)
C(4)-C(5)-Cl(3)	118.75(18)
C(5)-C(6)-C(7)	118.21(19)
C(5)-C(6)-Cl(4)	119.77(17)
C(7)-C(6)-Cl(4)	122.00(18)
N(1)-C(7)-C(2)	106.22(18)
N(1)-C(7)-C(6)	133.4(2)
C(2)-C(7)-C(6)	120.4(2)
N(1)-C(9)-C(10)	113.5(2)
C(11)-C(10)-C(19)	119.8(2)
C(11)-C(10)-C(9)	123.7(2)

C(19)-C(10)-C(9)	116.5(2)
C(10)-C(11)-C(12)	121.1(2)
C(13)-C(12)-C(17)	119.2(2)
C(13)-C(12)-C(11)	121.7(2)
C(17)-C(12)-C(11)	119.1(2)
C(14)-C(13)-C(12)	120.3(2)
C(13)-C(14)-C(15)	120.7(2)
C(16)-C(15)-C(14)	120.2(2)
C(15)-C(16)-C(17)	120.7(2)
C(18)-C(17)-C(16)	122.9(2)
C(18)-C(17)-C(12)	118.3(2)
C(16)-C(17)-C(12)	118.8(2)
C(19)-C(18)-C(17)	121.5(2)
C(18)-C(19)-C(10)	120.2(2)
O(2)-C(20)-O(1)	123.4(2)
O(2)-C(20)-C(21)	120.0(2)
O(1)-C(20)-C(21)	116.6(2)

Symmetry transformations used to generate equivalent atoms:

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

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)	22(1)	28(1)	20(1)	11(1)	7(1)	16(1)
Cl(1)	22(1)	18(1)	25(1)	13(1)	9(1)	10(1)
Cl(2)	20(1)	27(1)	22(1)	12(1)	7(1)	13(1)
Cl(3)	18(1)	23(1)	25(1)	9(1)	9(1)	4(1)
Cl(4)	32(1)	18(1)	32(1)	14(1)	18(1)	11(1)
O(1)	25(1)	32(1)	28(1)	20(1)	8(1)	14(1)
O(2)	33(1)	40(1)	45(1)	25(1)	8(1)	5(1)
O(3)	43(1)	32(1)	31(1)	12(1)	18(1)	9(1)
N(1)	26(1)	20(1)	18(1)	11(1)	11(1)	16(1)
N(2)	17(1)	19(1)	16(1)	8(1)	7(1)	10(1)
C(1)	22(1)	22(1)	16(1)	8(1)	11(1)	13(1)
C(2)	19(1)	17(1)	13(1)	5(1)	9(1)	9(1)
C(3)	22(1)	16(1)	17(1)	8(1)	11(1)	11(1)
C(4)	20(1)	21(1)	15(1)	8(1)	9(1)	13(1)
C(5)	18(1)	19(1)	17(1)	6(1)	10(1)	7(1)
C(6)	27(1)	14(1)	21(1)	8(1)	15(1)	10(1)
C(7)	23(1)	20(1)	14(1)	9(1)	10(1)	13(1)
C(8)	18(1)	19(1)	22(1)	9(1)	6(1)	8(1)
C(9)	32(1)	25(1)	20(1)	17(1)	15(1)	19(1)
C(10)	19(1)	15(1)	21(1)	9(1)	9(1)	9(1)
C(11)	20(1)	18(1)	19(1)	10(1)	8(1)	10(1)
C(12)	14(1)	17(1)	20(1)	8(1)	7(1)	6(1)
C(13)	17(1)	25(1)	21(1)	9(1)	6(1)	8(1)
C(14)	25(1)	26(1)	18(1)	5(1)	11(1)	8(1)
C(15)	28(1)	19(1)	33(2)	5(1)	17(1)	9(1)
C(16)	24(1)	18(1)	34(2)	12(1)	16(1)	10(1)
C(17)	17(1)	13(1)	24(1)	8(1)	9(1)	5(1)
C(18)	21(1)	15(1)	28(1)	13(1)	9(1)	10(1)
C(19)	24(1)	18(1)	18(1)	11(1)	9(1)	9(1)
C(20)	23(1)	28(1)	25(1)	12(1)	12(1)	15(1)
C(21)	31(1)	46(1)	31(1)	22(1)	14(1)	23(1)

C(22)	48(2)	36(1)	30(2)	15(1)	18(1)	19(1)

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

	x	y	z	U(eq)
H(3)	772	2233	2015	58
H(8A)	381	-2293	4494	30
H(8B)	1398	-2014	5896	30
H(8C)	1769	-2668	4735	30
H(9A)	2404	1979	3984	25
H(9B)	4232	2991	4835	25
H(11)	3506	3072	7265	21
H(13)	3458	4253	9328	27
H(14)	2988	5852	10564	31
H(15)	1998	7115	9723	34
H(16)	1478	6756	7646	30
H(18)	1497	5536	5561	25
H(19)	2094	4022	4354	24
H(21A)	-3433	231	413	50
H(21B)	-4496	-658	946	50
H(21C)	-4010	-1392	-92	50
H(22A)	1295	2906	570	57
H(22B)	1562	1627	581	57
H(22C)	3017	3159	1281	57

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