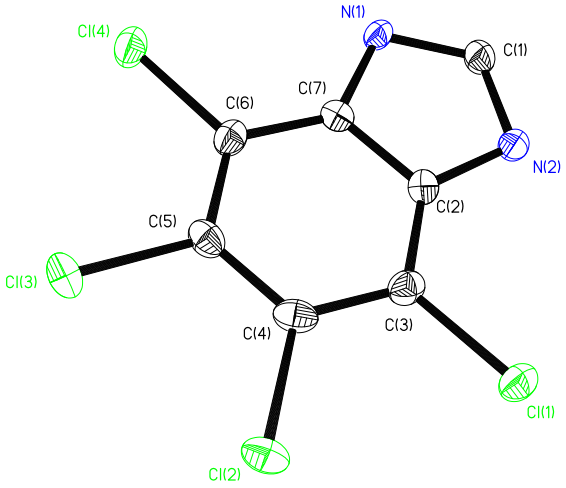
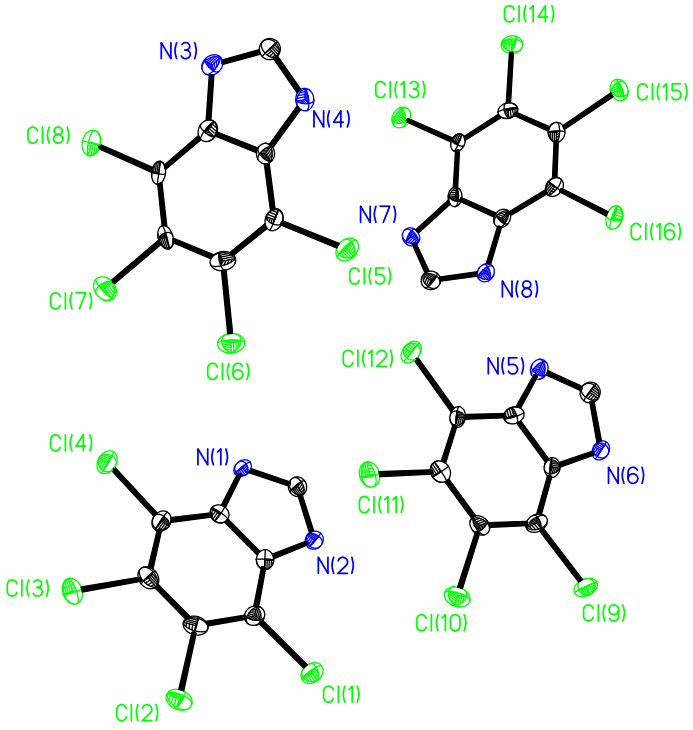


Molecule



Asym Unit

X-ray Structure Determination Details

A crystal of **$C_7H_2Cl_4N_2$** was coated in paraffin oil and mounted on a CryoLoop™ and placed on the goniometer head under a stream of nitrogen cooled to 100K. The data was collected on a Bruker APEX CCD diffractometer with graphite-monochromated Mo K_α radiation (λ = 0.71073 Å). The unit cell was determined by using reflections from three different orientations. The data was integrated using SAINT.[1] An empirical absorption correction and other corrections were applied to the data using multi-scan SADABS.[1] Structure solution, refinement, and modeling were accomplished by using the Bruker SHELXTL package.[1,2] The structure was determined by full-matrix least-squares refinement of F^2 and the selection of the appropriate atoms from the generated difference map. Hydrogen atom positions were calculated and U_{iso}(H) values were fixed according to a riding model.

Data collection was on March 13, 2009.

Table 1. Crystal data and structure refinement for bw.

Identification code	bw	
Empirical formula	C7 H2 Cl4 N2	
Formula weight	255.91	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.4984(19) Å	α= 108.611(4)°.
	b = 15.060(4) Å	β= 94.721(4)°.
	c = 16.612(4) Å	γ = 90.265(4)°.
Volume	1770.9(8) Å^3	
Z	8	
Density (calculated)	1.920 Mg/m^3	
Absorption coefficient	1.280 mm^{-1}	
F(000)	1008	
Crystal size	0.17 x 0.16 x 0.10 mm^3	
Theta range for data collection	1.30 to 26.30°.	
Index ranges	-9<=h<=9, -18<=k<=18, -20<=l<=20	
Reflections collected	13921	
Independent reflections	7025 [R(int) = 0.0275]	
Completeness to theta = 26.30°	97.7 %	
Absorption correction	Semi-empirical from equivalents	

[1] Bruker (1997). SMART (Version 5.625), SAINT (Version 6.22) and SHELXTL (Version 6.10)
[2] Sheldrick, G. M. (1997). SHELX-97. University of Göttingen, Germany

Max. and min. transmission	0.8827 and 0.7974
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7025 / 0 / 485
Goodness-of-fit on F^2	1.084
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.1055
R indices (all data)	R1 = 0.0449, wR2 = 0.1227
Largest diff. peak and hole	0.591 and -0.447 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)
Cl(1)	8912(1)	1912(1)	11239(1)	25(1)
Cl(2)	7177(1)	14(1)	11189(1)	24(1)
Cl(3)	6200(1)	-1550(1)	9454(1)	25(1)
Cl(4)	6911(1)	-1201(1)	7738(1)	26(1)
Cl(5)	1832(1)	2320(1)	6691(1)	25(1)
Cl(6)	3669(1)	670(1)	7160(1)	28(1)
Cl(7)	4159(1)	-1234(1)	5752(1)	27(1)
Cl(8)	2825(1)	-1492(1)	3834(1)	24(1)
Cl(9)	8458(1)	5999(1)	11331(1)	25(1)
Cl(10)	6754(1)	3996(1)	11070(1)	26(1)
Cl(11)	5397(1)	2701(1)	9253(1)	24(1)
Cl(12)	5929(1)	3346(1)	7657(1)	24(1)
Cl(13)	8722(1)	3316(1)	3398(1)	25(1)
Cl(14)	7037(1)	5119(1)	3112(1)	26(1)
Cl(15)	5841(1)	6737(1)	4648(1)	24(1)
Cl(16)	6332(1)	6578(1)	6509(1)	23(1)
N(1)	8857(3)	800(2)	8116(2)	18(1)
N(2)	9651(3)	1926(2)	9359(2)	19(1)
N(3)	995(3)	322(2)	3647(2)	19(1)
N(4)	576(3)	1686(2)	4661(2)	19(1)
N(5)	7627(3)	5386(2)	8202(2)	19(1)
N(6)	8541(3)	6348(2)	9513(2)	19(1)
N(7)	8943(3)	3462(2)	5362(2)	19(1)
N(8)	8011(3)	4621(2)	6452(2)	19(1)
C(1)	9646(4)	1655(2)	8519(2)	20(1)
C(2)	8810(4)	1180(2)	9517(2)	18(1)
C(3)	8421(4)	1046(2)	10280(2)	19(1)
C(4)	7618(4)	197(2)	10252(2)	20(1)
C(5)	7170(4)	-509(2)	9468(2)	20(1)
C(6)	7495(4)	-367(2)	8708(2)	19(1)
C(7)	8324(4)	478(2)	8743(2)	17(1)

C(8)	338(4)	1168(2)	3828(2)	20(1)
C(9)	1459(4)	1127(2)	5069(2)	17(1)
C(10)	2076(4)	1267(2)	5917(2)	18(1)
C(11)	2913(4)	528(2)	6115(2)	21(1)
C(12)	3147(4)	-330(2)	5480(2)	19(1)
C(13)	2558(4)	-455(2)	4637(2)	17(1)
C(14)	1712(4)	272(2)	4428(2)	18(1)
C(15)	8334(4)	6215(2)	8665(2)	22(1)
C(16)	7893(4)	5535(2)	9617(2)	18(1)
C(17)	7739(4)	5254(2)	10330(2)	19(1)
C(18)	6976(4)	4363(2)	10202(2)	18(1)
C(19)	6391(4)	3773(2)	9381(2)	19(1)
C(20)	6580(4)	4055(2)	8676(2)	18(1)
C(21)	7328(4)	4946(2)	8792(2)	18(1)
C(22)	8736(4)	3767(2)	6181(2)	21(1)
C(23)	8277(4)	4169(2)	5064(2)	17(1)
C(24)	8077(4)	4228(2)	4239(2)	16(1)
C(25)	7337(4)	5030(2)	4121(2)	18(1)
C(26)	6790(4)	5770(2)	4822(2)	20(1)
C(27)	6974(4)	5707(2)	5638(2)	18(1)
C(28)	7701(4)	4894(2)	5742(2)	17(1)

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

Cl(1)-C(3)	1.717(3)
Cl(2)-C(4)	1.723(3)
Cl(3)-C(5)	1.717(3)
Cl(4)-C(6)	1.719(3)
Cl(5)-C(10)	1.715(3)
Cl(6)-C(11)	1.726(3)
Cl(7)-C(12)	1.725(3)
Cl(8)-C(13)	1.725(3)
Cl(9)-C(17)	1.724(3)
Cl(10)-C(18)	1.720(3)
Cl(11)-C(19)	1.717(3)
Cl(12)-C(20)	1.717(3)
Cl(13)-C(24)	1.723(3)
Cl(14)-C(25)	1.719(3)
Cl(15)-C(26)	1.719(3)
Cl(16)-C(27)	1.719(3)
N(1)-C(1)	1.354(4)
N(1)-C(7)	1.368(4)
N(2)-C(1)	1.322(4)
N(2)-C(2)	1.393(4)
N(3)-C(8)	1.320(4)
N(3)-C(14)	1.387(4)
N(4)-C(8)	1.350(4)
N(4)-C(9)	1.379(4)
N(5)-C(15)	1.321(4)
N(5)-C(21)	1.378(4)
N(6)-C(15)	1.355(4)
N(6)-C(16)	1.380(4)
N(7)-C(22)	1.313(4)
N(7)-C(23)	1.389(4)
N(8)-C(22)	1.352(4)
N(8)-C(28)	1.370(4)
C(2)-C(7)	1.398(4)
C(2)-C(3)	1.399(4)

C(3)-C(4)	1.395(4)
C(4)-C(5)	1.407(4)
C(5)-C(6)	1.386(4)
C(6)-C(7)	1.396(4)
C(9)-C(10)	1.395(4)
C(9)-C(14)	1.411(4)
C(10)-C(11)	1.395(4)
C(11)-C(12)	1.406(4)
C(12)-C(13)	1.386(4)
C(13)-C(14)	1.392(4)
C(16)-C(17)	1.393(4)
C(16)-C(21)	1.403(4)
C(17)-C(18)	1.402(4)
C(18)-C(19)	1.403(4)
C(19)-C(20)	1.385(4)
C(20)-C(21)	1.401(4)
C(23)-C(24)	1.397(4)
C(23)-C(28)	1.396(4)
C(24)-C(25)	1.394(4)
C(25)-C(26)	1.422(4)
C(26)-C(27)	1.385(4)
C(27)-C(28)	1.396(4)

C(1)-N(1)-C(7)	106.1(3)
C(1)-N(2)-C(2)	104.0(2)
C(8)-N(3)-C(14)	104.3(2)
C(8)-N(4)-C(9)	106.0(2)
C(15)-N(5)-C(21)	104.2(2)
C(15)-N(6)-C(16)	106.0(3)
C(22)-N(7)-C(23)	104.1(2)
C(22)-N(8)-C(28)	105.9(2)
N(2)-C(1)-N(1)	114.1(3)
N(2)-C(2)-C(7)	109.3(2)
N(2)-C(2)-C(3)	131.3(3)
C(7)-C(2)-C(3)	119.4(3)
C(4)-C(3)-C(2)	119.0(3)

C(4)-C(3)-Cl(1)	120.3(2)
C(2)-C(3)-Cl(1)	120.7(2)
C(3)-C(4)-C(5)	120.9(3)
C(3)-C(4)-Cl(2)	119.4(2)
C(5)-C(4)-Cl(2)	119.7(2)
C(6)-C(5)-C(4)	120.4(3)
C(6)-C(5)-Cl(3)	119.9(2)
C(4)-C(5)-Cl(3)	119.8(2)
C(5)-C(6)-C(7)	118.4(3)
C(5)-C(6)-Cl(4)	121.7(2)
C(7)-C(6)-Cl(4)	119.9(2)
N(1)-C(7)-C(6)	131.6(3)
N(1)-C(7)-C(2)	106.4(2)
C(6)-C(7)-C(2)	122.0(3)
N(3)-C(8)-N(4)	114.5(3)
N(4)-C(9)-C(10)	133.2(3)
N(4)-C(9)-C(14)	105.8(3)
C(10)-C(9)-C(14)	121.0(3)
C(11)-C(10)-C(9)	118.0(3)
C(11)-C(10)-Cl(5)	121.0(2)
C(9)-C(10)-Cl(5)	120.9(2)
C(10)-C(11)-C(12)	121.2(3)
C(10)-C(11)-Cl(6)	119.3(2)
C(12)-C(11)-Cl(6)	119.5(2)
C(13)-C(12)-C(11)	120.3(3)
C(13)-C(12)-Cl(7)	119.9(2)
C(11)-C(12)-Cl(7)	119.9(2)
C(12)-C(13)-C(14)	119.4(3)
C(12)-C(13)-Cl(8)	122.0(2)
C(14)-C(13)-Cl(8)	118.6(2)
N(3)-C(14)-C(13)	130.6(3)
N(3)-C(14)-C(9)	109.3(3)
C(13)-C(14)-C(9)	120.1(3)
N(5)-C(15)-N(6)	114.2(3)
N(6)-C(16)-C(17)	133.0(3)
N(6)-C(16)-C(21)	105.5(3)

C(17)-C(16)-C(21)	121.5(3)
C(16)-C(17)-C(18)	117.9(3)
C(16)-C(17)-Cl(9)	120.0(2)
C(18)-C(17)-Cl(9)	122.1(2)
C(17)-C(18)-C(19)	120.9(3)
C(17)-C(18)-Cl(10)	119.1(2)
C(19)-C(18)-Cl(10)	119.9(2)
C(20)-C(19)-C(18)	120.5(3)
C(20)-C(19)-Cl(11)	119.9(2)
C(18)-C(19)-Cl(11)	119.6(2)
C(19)-C(20)-C(21)	119.3(3)
C(19)-C(20)-Cl(12)	122.1(2)
C(21)-C(20)-Cl(12)	118.6(2)
N(5)-C(21)-C(20)	130.1(3)
N(5)-C(21)-C(16)	110.1(3)
C(20)-C(21)-C(16)	119.8(3)
N(7)-C(22)-N(8)	114.4(3)
N(7)-C(23)-C(24)	130.7(3)
N(7)-C(23)-C(28)	109.4(3)
C(24)-C(23)-C(28)	119.8(3)
C(25)-C(24)-C(23)	118.5(3)
C(25)-C(24)-Cl(13)	121.7(2)
C(23)-C(24)-Cl(13)	119.8(2)
C(24)-C(25)-C(26)	120.8(3)
C(24)-C(25)-Cl(14)	119.8(2)
C(26)-C(25)-Cl(14)	119.4(2)
C(27)-C(26)-C(25)	120.6(3)
C(27)-C(26)-Cl(15)	119.9(2)
C(25)-C(26)-Cl(15)	119.5(2)
C(26)-C(27)-C(28)	117.7(3)
C(26)-C(27)-Cl(16)	122.6(2)
C(28)-C(27)-Cl(16)	119.7(2)
N(8)-C(28)-C(27)	131.3(3)
N(8)-C(28)-C(23)	106.2(2)
C(27)-C(28)-C(23)	122.5(3)

Symmetry transformations used to generate equivalent atoms:

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}
Cl(1)	32(1)	23(1)	17(1)	3(1)	3(1)	-2(1)
Cl(2)	26(1)	30(1)	21(1)	14(1)	6(1)	3(1)
Cl(3)	27(1)	19(1)	31(1)	12(1)	5(1)	-2(1)
Cl(4)	34(1)	20(1)	21(1)	3(1)	1(1)	-7(1)
Cl(5)	31(1)	22(1)	17(1)	2(1)	2(1)	-2(1)
Cl(6)	33(1)	34(1)	18(1)	11(1)	-2(1)	-3(1)
Cl(7)	25(1)	25(1)	33(1)	14(1)	1(1)	3(1)
Cl(8)	27(1)	17(1)	26(1)	2(1)	5(1)	0(1)
Cl(9)	30(1)	27(1)	14(1)	3(1)	-1(1)	2(1)
Cl(10)	32(1)	30(1)	21(1)	14(1)	5(1)	5(1)
Cl(11)	26(1)	19(1)	29(1)	10(1)	5(1)	-1(1)
Cl(12)	31(1)	19(1)	17(1)	1(1)	1(1)	-6(1)
Cl(13)	33(1)	22(1)	16(1)	1(1)	7(1)	2(1)
Cl(14)	35(1)	27(1)	17(1)	10(1)	0(1)	-1(1)
Cl(15)	27(1)	18(1)	28(1)	10(1)	2(1)	1(1)
Cl(16)	29(1)	16(1)	22(1)	0(1)	6(1)	2(1)
N(1)	24(1)	16(1)	12(1)	2(1)	0(1)	-3(1)
N(2)	23(1)	17(1)	16(1)	5(1)	1(1)	-3(1)
N(3)	21(1)	21(1)	15(1)	4(1)	3(1)	-4(1)
N(4)	22(1)	15(1)	20(1)	6(1)	5(1)	0(1)
N(5)	25(1)	15(1)	17(1)	5(1)	4(1)	-3(1)
N(6)	25(1)	15(1)	16(1)	3(1)	2(1)	-2(1)
N(7)	24(1)	17(1)	18(1)	8(1)	3(1)	0(1)
N(8)	27(1)	16(1)	14(1)	3(1)	3(1)	0(1)
C(1)	25(2)	18(2)	19(2)	7(1)	3(1)	-3(1)
C(2)	18(1)	15(1)	19(2)	5(1)	2(1)	0(1)
C(3)	21(2)	20(2)	17(2)	4(1)	2(1)	4(1)
C(4)	17(1)	28(2)	18(2)	12(1)	4(1)	3(1)
C(5)	17(1)	21(2)	24(2)	12(1)	4(1)	-1(1)
C(6)	20(2)	17(2)	18(2)	2(1)	1(1)	0(1)
C(7)	17(1)	18(2)	17(2)	7(1)	2(1)	1(1)

C(8)	23(2)	20(2)	18(2)	8(1)	3(1)	-3(1)
C(9)	17(1)	15(1)	19(1)	6(1)	2(1)	-3(1)
C(10)	22(2)	15(1)	17(2)	2(1)	4(1)	-3(1)
C(11)	19(2)	30(2)	16(2)	10(1)	1(1)	-5(1)
C(12)	19(1)	12(1)	29(2)	9(1)	2(1)	0(1)
C(13)	19(1)	9(1)	20(2)	2(1)	5(1)	-2(1)
C(14)	18(1)	18(1)	17(1)	5(1)	5(1)	-5(1)
C(15)	26(2)	21(2)	21(2)	7(1)	4(1)	-1(1)
C(16)	19(1)	13(1)	19(2)	3(1)	1(1)	3(1)
C(17)	17(1)	24(2)	14(1)	2(1)	2(1)	3(1)
C(18)	20(1)	19(2)	18(2)	10(1)	7(1)	5(1)
C(19)	16(1)	19(2)	23(2)	9(1)	4(1)	2(1)
C(20)	21(2)	12(1)	19(2)	2(1)	2(1)	2(1)
C(21)	16(1)	21(2)	14(1)	4(1)	0(1)	0(1)
C(22)	23(2)	21(2)	18(2)	7(1)	2(1)	-1(1)
C(23)	22(2)	11(1)	18(1)	4(1)	5(1)	-2(1)
C(24)	18(1)	12(1)	15(1)	1(1)	2(1)	-2(1)
C(25)	18(1)	22(2)	14(1)	7(1)	-1(1)	-4(1)
C(26)	21(2)	16(1)	22(2)	5(1)	2(1)	-1(1)
C(27)	16(1)	18(1)	17(1)	2(1)	3(1)	-1(1)
C(28)	18(1)	15(1)	16(1)	3(1)	2(1)	-4(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(1)	10151	2028	8224	25
H(8)	-253	1393	3408	24
H(15)	8668	6677	8423	26
H(22)	9067	3418	6553	25
H(2)	8870(40)	570(20)	7660(20)	14(9)
H(3)	100(60)	2230(30)	4850(30)	48(12)
H(4)	9020(50)	6850(30)	9910(20)	34(10)
H(5)	7860(50)	4890(30)	6990(30)	42(12)

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