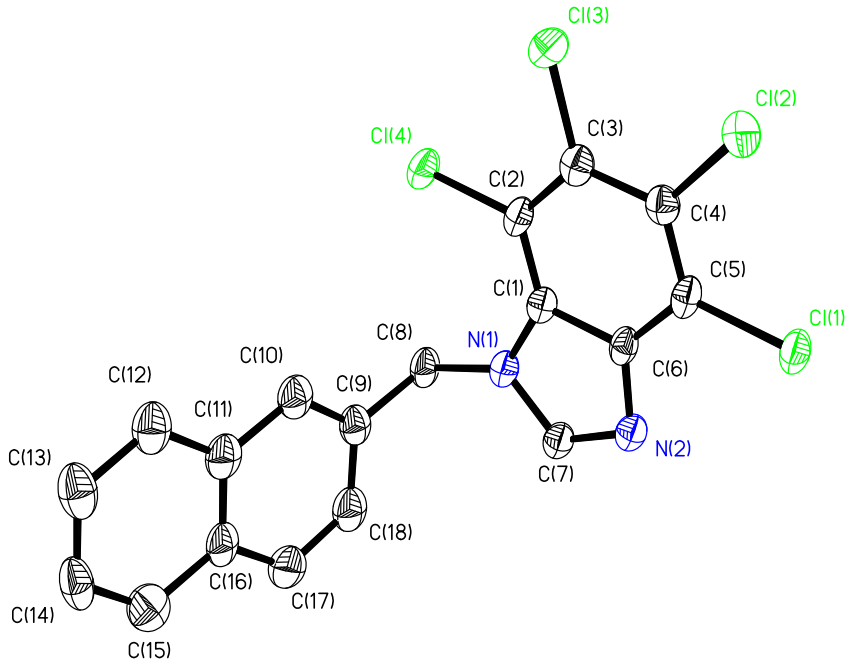

Asymmetric unit drawn with thermal ellipsoids at 50% probability.

X-ray Structure Determination Details

A crystal of $\mathbf{C_{18}H_{10}N_2Cl_4}$ 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 ($\lambda = 0.71073$ 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 3, 2010.

[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

Table 1. Crystal data and structure refinement for bw.

Identification code	bw	
Empirical formula	C18 H10 Cl4 N2	
Formula weight	396.08	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 4.979(5) Å	α= 84.139(16)°.
	b = 12.523(13) Å	β= 87.926(16)°.
	c = 13.184(13) Å	γ = 83.410(16)°.
Volume	812.1(14) $Å^3$	
Z	2	
Density (calculated)	1.620 Mg/m^3	
Absorption coefficient	0.730 mm^{-1}	
F(000)	400	
Crystal size	0.37 x 0.07 x 0.07 mm^3	
Theta range for data collection	1.55 to 26.30°.	
Index ranges	-6<=h<=6, -15<=k<=15, -16<=l<=16	
Reflections collected	6080	
Independent reflections	3170 [R(int) = 0.0531]	
Completeness to theta = 26.30°	96.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9520 and 0.7729	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3170 / 0 / 217	
Goodness-of-fit on F^2	0.937	
Final R indices [I>2sigma(I)]	R1 = 0.0596, wR2 = 0.1484	
R indices (all data)	R1 = 0.0830, wR2 = 0.1622	
Largest diff. peak and hole	0.667 and -0.587 $e.Å^{-3}$	

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)	1764(2)	1796(1)	9072(1)	33(1)
Cl(2)	2132(2)	182(1)	11020(1)	33(1)
Cl(3)	5912(2)	452(1)	12784(1)	35(1)
Cl(4)	9190(2)	2484(1)	12679(1)	33(1)
N(1)	5764(6)	3697(3)	9268(2)	27(1)
N(2)	8411(6)	3891(3)	10587(2)	28(1)
C(1)	5370(6)	2850(3)	9997(3)	24(1)
C(2)	3821(7)	1988(3)	10057(3)	27(1)
C(3)	3998(7)	1268(3)	10929(3)	27(1)
C(4)	5666(7)	1409(3)	11743(3)	27(1)
C(5)	7160(7)	2274(3)	11693(3)	27(1)
C(6)	7033(7)	2999(3)	10817(3)	26(1)
C(7)	7590(7)	4275(3)	9667(3)	29(1)
C(8)	4660(7)	3974(3)	8239(3)	32(1)
C(9)	6796(7)	3743(3)	7421(3)	31(1)
C(10)	7317(7)	2749(4)	7086(3)	37(1)
C(11)	9386(8)	2537(4)	6315(3)	36(1)
C(12)	9914(8)	1526(4)	5944(3)	42(1)
C(13)	11883(8)	1370(4)	5199(3)	45(1)
C(14)	13398(8)	2199(4)	4795(3)	43(1)
C(15)	12917(8)	3190(4)	5142(3)	46(1)
C(16)	10837(8)	3404(4)	5917(3)	35(1)
C(17)	10263(8)	4420(4)	6272(3)	41(1)
C(18)	8272(8)	4596(4)	6998(3)	40(1)

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

Cl(1)-C(2)	1.735(4)
Cl(2)-C(3)	1.725(4)
Cl(3)-C(4)	1.725(4)
Cl(4)-C(5)	1.735(4)
N(1)-C(7)	1.375(5)
N(1)-C(1)	1.384(5)
N(1)-C(8)	1.475(4)
N(2)-C(7)	1.320(5)
N(2)-C(6)	1.380(5)
C(1)-C(2)	1.391(5)
C(1)-C(6)	1.425(5)
C(2)-C(3)	1.386(5)
C(3)-C(4)	1.418(5)
C(4)-C(5)	1.377(5)
C(5)-C(6)	1.393(5)
C(8)-C(9)	1.513(5)
C(9)-C(10)	1.357(6)
C(9)-C(18)	1.421(6)
C(10)-C(11)	1.443(5)
C(11)-C(12)	1.397(6)
C(11)-C(16)	1.418(6)
C(12)-C(13)	1.374(5)
C(13)-C(14)	1.404(7)
C(14)-C(15)	1.359(7)
C(15)-C(16)	1.451(6)
C(16)-C(17)	1.396(6)
C(17)-C(18)	1.369(6)

C(7)-N(1)-C(1)	106.1(3)
C(7)-N(1)-C(8)	123.1(3)
C(1)-N(1)-C(8)	130.8(3)
C(7)-N(2)-C(6)	103.7(3)
N(1)-C(1)-C(2)	134.5(3)
N(1)-C(1)-C(6)	104.6(3)

C(2)-C(1)-C(6)	121.0(3)
C(3)-C(2)-C(1)	117.8(3)
C(3)-C(2)-Cl(1)	120.4(3)
C(1)-C(2)-Cl(1)	121.8(3)
C(2)-C(3)-C(4)	121.4(4)
C(2)-C(3)-Cl(2)	118.9(3)
C(4)-C(3)-Cl(2)	119.7(3)
C(5)-C(4)-C(3)	120.8(3)
C(5)-C(4)-Cl(3)	120.0(3)
C(3)-C(4)-Cl(3)	119.1(3)
C(4)-C(5)-C(6)	118.6(3)
C(4)-C(5)-Cl(4)	122.2(3)
C(6)-C(5)-Cl(4)	119.2(3)
N(2)-C(6)-C(5)	128.6(3)
N(2)-C(6)-C(1)	111.0(3)
C(5)-C(6)-C(1)	120.4(3)
N(2)-C(7)-N(1)	114.6(4)
N(1)-C(8)-C(9)	111.3(3)
C(10)-C(9)-C(18)	119.9(4)
C(10)-C(9)-C(8)	121.6(4)
C(18)-C(9)-C(8)	118.5(4)
C(9)-C(10)-C(11)	120.9(4)
C(12)-C(11)-C(16)	120.4(4)
C(12)-C(11)-C(10)	121.9(4)
C(16)-C(11)-C(10)	117.7(4)
C(13)-C(12)-C(11)	119.6(4)
C(12)-C(13)-C(14)	121.9(5)
C(15)-C(14)-C(13)	119.6(4)
C(14)-C(15)-C(16)	120.8(4)
C(17)-C(16)-C(11)	120.4(4)
C(17)-C(16)-C(15)	121.9(4)
C(11)-C(16)-C(15)	117.7(4)
C(18)-C(17)-C(16)	120.4(4)
C(17)-C(18)-C(9)	120.7(4)

Symmetry transformations used to generate equivalent atoms:

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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)	30(1)	39(1)	31(1)	-12(1)	-9(1)	-3(1)
Cl(2)	31(1)	33(1)	38(1)	-10(1)	-3(1)	-5(1)
Cl(3)	38(1)	37(1)	28(1)	-3(1)	-3(1)	-2(1)
Cl(4)	33(1)	45(1)	24(1)	-10(1)	-8(1)	-3(1)
N(1)	28(2)	30(2)	24(2)	-7(1)	-5(1)	0(1)
N(2)	27(2)	30(2)	27(2)	-8(1)	-3(1)	-1(1)
C(1)	22(2)	26(2)	24(2)	-7(2)	-4(1)	2(1)
C(2)	21(2)	34(2)	27(2)	-14(2)	-5(1)	2(2)
C(3)	23(2)	29(2)	29(2)	-11(2)	0(1)	6(2)
C(4)	23(2)	33(2)	25(2)	-5(2)	0(1)	2(2)
C(5)	22(2)	34(2)	25(2)	-13(2)	-6(1)	5(2)
C(6)	22(2)	31(2)	24(2)	-13(2)	-3(1)	3(2)
C(7)	30(2)	32(2)	27(2)	-9(2)	-3(1)	-3(2)
C(8)	30(2)	42(3)	24(2)	-7(2)	-9(2)	2(2)
C(9)	29(2)	40(3)	24(2)	-4(2)	-8(1)	3(2)
C(10)	32(2)	50(3)	29(2)	-8(2)	-10(2)	1(2)
C(11)	36(2)	45(3)	28(2)	-5(2)	-13(2)	1(2)
C(12)	43(2)	48(3)	34(2)	-9(2)	-10(2)	6(2)
C(13)	45(2)	58(3)	30(2)	-8(2)	-6(2)	11(2)
C(14)	36(2)	66(3)	25(2)	-12(2)	-5(2)	11(2)
C(15)	40(2)	62(3)	34(2)	-2(2)	-13(2)	-1(2)
C(16)	34(2)	47(3)	24(2)	-7(2)	-12(2)	2(2)
C(17)	42(2)	49(3)	33(2)	-3(2)	-11(2)	-6(2)
C(18)	40(2)	51(3)	30(2)	-7(2)	-12(2)	1(2)

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

	x	y	z	U(eq)
H(7)	8210	4901	9309	35
H(8A)	3961	4750	8155	38
H(8B)	3133	3550	8162	38
H(10)	6305	2185	7363	44
H(12)	8919	951	6204	51
H(13)	12230	680	4951	54
H(14)	14751	2069	4281	51
H(15)	13956	3749	4874	55
H(17)	11261	4994	6007	50
H(18)	7872	5295	7223	48

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