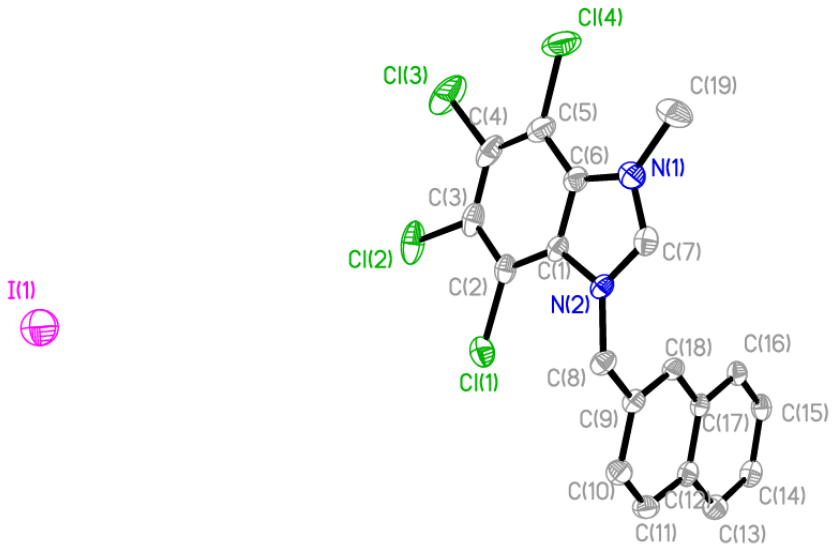

Asymmetric unit of $C_{19}H_{13}N_2Cl_4I_1$ with thermal ellipsoids drawn at 50% probability.

X-ray Structure Determination Details

A crystal of **$C_{19}H_{13}N_2Cl_4I_1$** 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 May 5, 2011.

[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	C19 H13 Cl4 I N2	
Formula weight	538.01	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 24.500(3) Å	α= 90°.
	b = 12.9443(12) Å	β= 117.003(2)°.
	c = 14.1288(13) Å	γ = 90°.
Volume	3992.3(7) $Å^3$	
Z	8	
Density (calculated)	1.790 Mg/m^3	
Absorption coefficient	2.146 mm^{-1}	
F(000)	2096	
Crystal size	0.26 x 0.15 x 0.08 mm^3	
Theta range for data collection	1.83 to 27.51°.	
Index ranges	-31<=h<=31, -16<=k<=16, -18<=l<=18	
Reflections collected	17009	
Independent reflections	4569 [R(int) = 0.0396]	
Completeness to theta = 27.51°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8522 and 0.6086	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4569 / 0 / 236	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0798	
R indices (all data)	R1 = 0.0404, wR2 = 0.0850	
Largest diff. peak and hole	1.358 and -0.515 $e.Å^{-3}$	

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)
I(1)	1298(1)	662(1)	9991(1)	27(1)
Cl(1)	2956(1)	7001(1)	2118(1)	31(1)
Cl(2)	2219(1)	5999(1)	-84(1)	43(1)
Cl(4)	137(1)	7849(1)	-500(1)	51(1)
Cl(3)	820(1)	6382(1)	-1378(1)	58(1)
N(2)	2081(1)	8485(2)	2710(2)	19(1)
N(1)	1097(1)	8789(2)	1790(2)	26(1)
C(9)	3135(1)	9171(2)	3404(2)	21(1)
C(17)	3365(1)	10492(2)	2431(2)	19(1)
C(12)	3996(1)	10376(2)	3102(2)	23(1)
C(13)	4419(1)	11006(2)	2936(2)	26(1)
C(2)	2191(1)	7262(2)	1394(2)	24(1)
C(16)	3165(1)	11216(2)	1586(2)	22(1)
C(3)	1851(2)	6803(2)	416(2)	30(1)
C(11)	4190(1)	9608(2)	3913(2)	26(1)
C(5)	910(2)	7641(3)	203(2)	32(1)
C(1)	1880(1)	7915(2)	1769(2)	21(1)
C(10)	3770(1)	9025(2)	4059(2)	26(1)
C(4)	1219(2)	6986(3)	-173(2)	34(1)
C(15)	3578(1)	11813(2)	1435(2)	23(1)
C(18)	2938(1)	9880(2)	2603(2)	20(1)
C(7)	1601(1)	8991(2)	2678(2)	23(1)
C(14)	4207(1)	11713(2)	2118(2)	26(1)
C(6)	1256(1)	8109(2)	1188(2)	24(1)
C(8)	2691(1)	8526(2)	3625(2)	23(1)
C(19)	502(2)	9275(3)	1540(3)	38(1)

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

Cl(1)-C(2)	1.711(3)
Cl(2)-C(3)	1.724(3)
Cl(4)-C(5)	1.715(3)
Cl(3)-C(4)	1.719(3)
N(2)-C(7)	1.329(4)
N(2)-C(1)	1.400(3)
N(2)-C(8)	1.467(3)
N(1)-C(7)	1.326(4)
N(1)-C(6)	1.396(4)
N(1)-C(19)	1.476(4)
C(9)-C(18)	1.363(4)
C(9)-C(10)	1.416(4)
C(9)-C(8)	1.513(4)
C(17)-C(12)	1.407(4)
C(17)-C(16)	1.418(4)
C(17)-C(18)	1.420(4)
C(12)-C(13)	1.420(4)
C(12)-C(11)	1.425(4)
C(13)-C(14)	1.377(4)
C(2)-C(3)	1.382(4)
C(2)-C(1)	1.393(4)
C(16)-C(15)	1.364(4)
C(3)-C(4)	1.406(5)
C(11)-C(10)	1.364(4)
C(5)-C(4)	1.392(5)
C(5)-C(6)	1.397(4)
C(1)-C(6)	1.391(4)
C(15)-C(14)	1.405(4)

C(7)-N(2)-C(1)	107.7(2)
C(7)-N(2)-C(8)	123.0(2)
C(1)-N(2)-C(8)	129.3(2)
C(7)-N(1)-C(6)	107.7(2)
C(7)-N(1)-C(19)	122.4(3)

C(6)-N(1)-C(19)	129.9(3)
C(18)-C(9)-C(10)	120.2(3)
C(18)-C(9)-C(8)	121.6(3)
C(10)-C(9)-C(8)	118.1(3)
C(12)-C(17)-C(16)	119.5(3)
C(12)-C(17)-C(18)	119.6(3)
C(16)-C(17)-C(18)	120.9(3)
C(17)-C(12)-C(13)	119.2(3)
C(17)-C(12)-C(11)	118.7(3)
C(13)-C(12)-C(11)	122.1(3)
C(14)-C(13)-C(12)	119.8(3)
C(3)-C(2)-C(1)	117.1(3)
C(3)-C(2)-Cl(1)	120.8(2)
C(1)-C(2)-Cl(1)	122.1(2)
C(15)-C(16)-C(17)	120.6(3)
C(2)-C(3)-C(4)	121.5(3)
C(2)-C(3)-Cl(2)	118.6(3)
C(4)-C(3)-Cl(2)	119.9(2)
C(10)-C(11)-C(12)	120.5(3)
C(4)-C(5)-C(6)	117.1(3)
C(4)-C(5)-Cl(4)	121.5(2)
C(6)-C(5)-Cl(4)	121.3(3)
C(6)-C(1)-C(2)	122.0(3)
C(6)-C(1)-N(2)	106.4(2)
C(2)-C(1)-N(2)	131.6(3)
C(11)-C(10)-C(9)	120.5(3)
C(5)-C(4)-C(3)	121.3(3)
C(5)-C(4)-Cl(3)	119.5(3)
C(3)-C(4)-Cl(3)	119.2(3)
C(16)-C(15)-C(14)	120.1(3)
C(9)-C(18)-C(17)	120.4(3)
N(1)-C(7)-N(2)	111.3(3)
C(13)-C(14)-C(15)	120.9(3)
C(1)-C(6)-C(5)	121.1(3)
C(1)-C(6)-N(1)	106.9(2)
C(5)-C(6)-N(1)	132.0(3)

N(2)-C(8)-C(9)	112.3(2)

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}
I(1)	27(1)	30(1)	25(1)	5(1)	12(1)	-3(1)
Cl(1)	35(1)	26(1)	37(1)	1(1)	20(1)	5(1)
Cl(2)	83(1)	24(1)	39(1)	-6(1)	43(1)	-4(1)
Cl(4)	32(1)	53(1)	43(1)	5(1)	-4(1)	-12(1)
Cl(3)	80(1)	55(1)	25(1)	-17(1)	11(1)	-26(1)
N(2)	23(1)	19(1)	17(1)	0(1)	9(1)	-5(1)
N(1)	25(1)	25(1)	32(1)	6(1)	16(1)	0(1)
C(9)	23(1)	20(1)	19(1)	-2(1)	10(1)	-3(1)
C(17)	23(1)	17(1)	20(1)	-4(1)	11(1)	0(1)
C(12)	26(2)	20(1)	24(1)	-5(1)	14(1)	-1(1)
C(13)	24(1)	29(2)	29(2)	-3(1)	14(1)	-1(1)
C(2)	35(2)	17(1)	24(1)	2(1)	17(1)	-2(1)
C(16)	26(1)	18(1)	22(1)	-1(1)	12(1)	2(1)
C(3)	50(2)	20(1)	26(2)	-2(1)	23(2)	-6(1)
C(11)	21(1)	28(2)	26(2)	1(1)	8(1)	-2(1)
C(5)	31(2)	30(2)	25(2)	3(1)	4(1)	-9(1)
C(1)	28(1)	18(1)	16(1)	0(1)	10(1)	-4(1)
C(10)	29(2)	25(2)	21(1)	3(1)	8(1)	-1(1)
C(4)	51(2)	27(2)	20(2)	-5(1)	11(1)	-15(2)
C(15)	32(2)	19(1)	24(1)	0(1)	17(1)	2(1)
C(18)	21(1)	21(1)	18(1)	-4(1)	8(1)	-1(1)
C(7)	29(2)	20(1)	26(2)	1(1)	18(1)	-3(1)
C(14)	30(2)	23(1)	32(2)	-4(1)	21(1)	-4(1)
C(6)	27(2)	20(1)	25(1)	4(1)	11(1)	-5(1)
C(8)	25(1)	23(1)	18(1)	-1(1)	9(1)	-5(1)
C(19)	26(2)	46(2)	45(2)	12(2)	18(2)	6(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(13)	4837	10942	3377	31
H(16)	2749	11284	1131	26
H(11)	4606	9503	4346	32
H(10)	3902	8529	4593	31
H(15)	3442	12286	880	27
H(18)	2520	9962	2167	24
H(7)	1616	9431	3210	28
H(14)	4485	12131	2017	31
H(8A)	2850	7829	3809	27
H(8B)	2656	8814	4229	27
H(19A)	536	9664	2143	58
H(19B)	196	8749	1373	58
H(19C)	388	9728	942	58

Electronic Supplementary Material (ESI) for Dalton Transactions