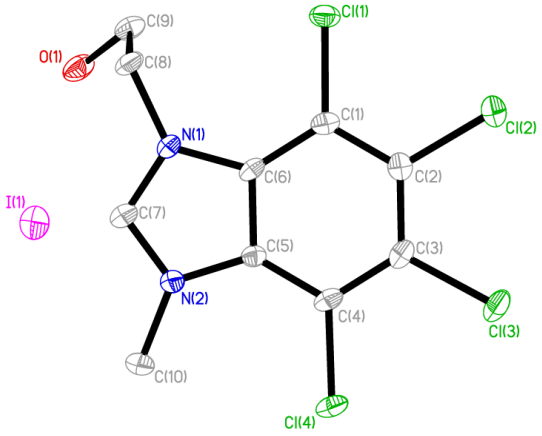

Asymmetric Unit with thermal ellipsoids drawn to 50% probability.

X-ray Structure Determination Details

A crystal of $C_{10}H_9N_2Cl_4O_1I_1$ 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 February 14, 2011.

Table 1. Crystal data and structure refinement for bw.

Identification code	bw
Empirical formula	C10 H9 Cl4 I N2 O
Formula weight	441.89
Temperature	100(2) K
Wavelength	0.71073 Å

[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

Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.2405(9) Å	α= 90°.
	b = 6.9153(7) Å	β= 99.331(2)°.
	c = 22.244(2) Å	γ = 90°.
Volume	1402.6(2) $Å^3$	
Z	4	
Density (calculated)	2.093 Mg/m^3	
Absorption coefficient	3.033 mm^{-1}	
F(000)	848	
Crystal size	0.23 x 0.11 x 0.08 mm^3	
Theta range for data collection	1.86 to 28.33°.	
Index ranges	-11<=h<=12, -9<=k<=9, -28<=l<=29	
Reflections collected	11737	
Independent reflections	3346 [R(int) = 0.0311]	
Completeness to theta = 28.33°	95.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7934 and 0.6324	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3346 / 0 / 165	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0257, wR2 = 0.0630	
R indices (all data)	R1 = 0.0276, wR2 = 0.0639	
Largest diff. peak and hole	1.955 and -0.405 $e.Å^{-3}$	

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)	1188(1)	1798(1)	3198(1)	21(1)
Cl(1)	6058(1)	7231(1)	4364(1)	21(1)
Cl(2)	5682(1)	7795(1)	5711(1)	22(1)
Cl(3)	2587(1)	7840(1)	6080(1)	25(1)
Cl(4)	-211(1)	7519(1)	5107(1)	22(1)
O(1)	3440(2)	9084(3)	2415(1)	28(1)
N(1)	2865(2)	6728(3)	3499(1)	15(1)
N(2)	682(2)	6946(3)	3754(1)	15(1)
C(1)	1425(3)	6679(3)	3299(1)	16(1)
C(2)	1676(3)	7192(3)	4285(1)	15(1)
C(3)	3077(3)	7064(3)	4122(1)	15(1)
C(4)	4329(3)	7277(3)	4558(1)	16(1)
C(5)	4155(3)	7551(3)	5158(1)	17(1)
C(6)	2748(3)	7625(4)	5324(1)	18(1)
C(7)	1496(3)	7453(3)	4892(1)	16(1)
C(8)	-928(3)	7041(4)	3656(1)	23(1)
C(9)	3951(3)	6328(4)	3094(1)	20(1)
C(10)	4523(3)	8160(4)	2844(1)	23(1)

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

Cl(1)-C(4)	1.722(2)
Cl(2)-C(5)	1.723(3)
Cl(3)-C(6)	1.720(3)
Cl(4)-C(7)	1.721(2)
O(1)-C(10)	1.418(3)
N(1)-C(1)	1.333(3)
N(1)-C(3)	1.386(3)
N(1)-C(9)	1.479(3)
N(2)-C(1)	1.324(3)
N(2)-C(2)	1.385(3)
N(2)-C(8)	1.469(3)
C(2)-C(7)	1.398(3)
C(2)-C(3)	1.404(3)
C(3)-C(4)	1.392(4)
C(4)-C(5)	1.384(3)
C(5)-C(6)	1.409(4)
C(6)-C(7)	1.384(4)
C(9)-C(10)	1.513(4)

C(1)-N(1)-C(3)	108.1(2)
C(1)-N(1)-C(9)	122.0(2)
C(3)-N(1)-C(9)	129.7(2)
C(1)-N(2)-C(2)	108.4(2)
C(1)-N(2)-C(8)	122.1(2)
C(2)-N(2)-C(8)	129.4(2)
N(2)-C(1)-N(1)	110.7(2)
N(2)-C(2)-C(7)	132.4(2)
N(2)-C(2)-C(3)	106.4(2)
C(7)-C(2)-C(3)	121.2(2)
N(1)-C(3)-C(4)	133.0(2)
N(1)-C(3)-C(2)	106.4(2)
C(4)-C(3)-C(2)	120.7(2)
C(5)-C(4)-C(3)	118.3(2)
C(5)-C(4)-Cl(1)	120.18(19)

C(3)-C(4)-Cl(1)	121.54(19)
C(4)-C(5)-C(6)	120.9(2)
C(4)-C(5)-Cl(2)	119.50(19)
C(6)-C(5)-Cl(2)	119.57(19)
C(7)-C(6)-C(5)	121.2(2)
C(7)-C(6)-Cl(3)	119.46(19)
C(5)-C(6)-Cl(3)	119.25(19)
C(6)-C(7)-C(2)	117.7(2)
C(6)-C(7)-Cl(4)	120.35(19)
C(2)-C(7)-Cl(4)	121.98(19)
N(1)-C(9)-C(10)	112.3(2)
O(1)-C(10)-C(9)	112.0(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)	24(1)	16(1)	21(1)	-1(1)	-1(1)	0(1)
Cl(1)	14(1)	23(1)	28(1)	2(1)	4(1)	0(1)
Cl(2)	23(1)	19(1)	21(1)	1(1)	-4(1)	-1(1)
Cl(3)	35(1)	26(1)	17(1)	-2(1)	8(1)	-5(1)
Cl(4)	21(1)	20(1)	27(1)	-1(1)	12(1)	0(1)
O(1)	32(1)	31(1)	24(1)	7(1)	10(1)	6(1)
N(1)	14(1)	15(1)	17(1)	-1(1)	4(1)	-1(1)
N(2)	15(1)	14(1)	17(1)	0(1)	2(1)	-1(1)
C(1)	19(1)	13(1)	17(1)	0(1)	3(1)	1(1)
C(2)	13(1)	12(1)	20(1)	0(1)	3(1)	0(1)
C(3)	18(1)	10(1)	17(1)	1(1)	5(1)	0(1)
C(4)	16(1)	14(1)	20(1)	1(1)	5(1)	1(1)
C(5)	20(1)	12(1)	18(1)	1(1)	0(1)	-1(1)
C(6)	25(1)	13(1)	17(1)	-1(1)	6(1)	-1(1)
C(7)	19(1)	11(1)	20(1)	1(1)	8(1)	0(1)
C(8)	14(1)	29(1)	26(1)	0(1)	3(1)	-1(1)
C(9)	20(1)	21(1)	21(1)	-1(1)	9(1)	1(1)
C(10)	23(1)	23(1)	26(1)	4(1)	11(1)	0(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)	2917	9791	2599	43
H(1A)	991	6480	2886	20
H(8A)	-1306	6954	3219	34
H(8B)	-1237	8269	3815	34
H(8C)	-1313	5965	3869	34
H(9A)	3491	5508	2751	24
H(9B)	4784	5599	3324	24
H(10A)	4855	9061	3185	28
H(10B)	5379	7842	2647	28

Electronic Supplementary Material (ESI) for Dalton Transactions