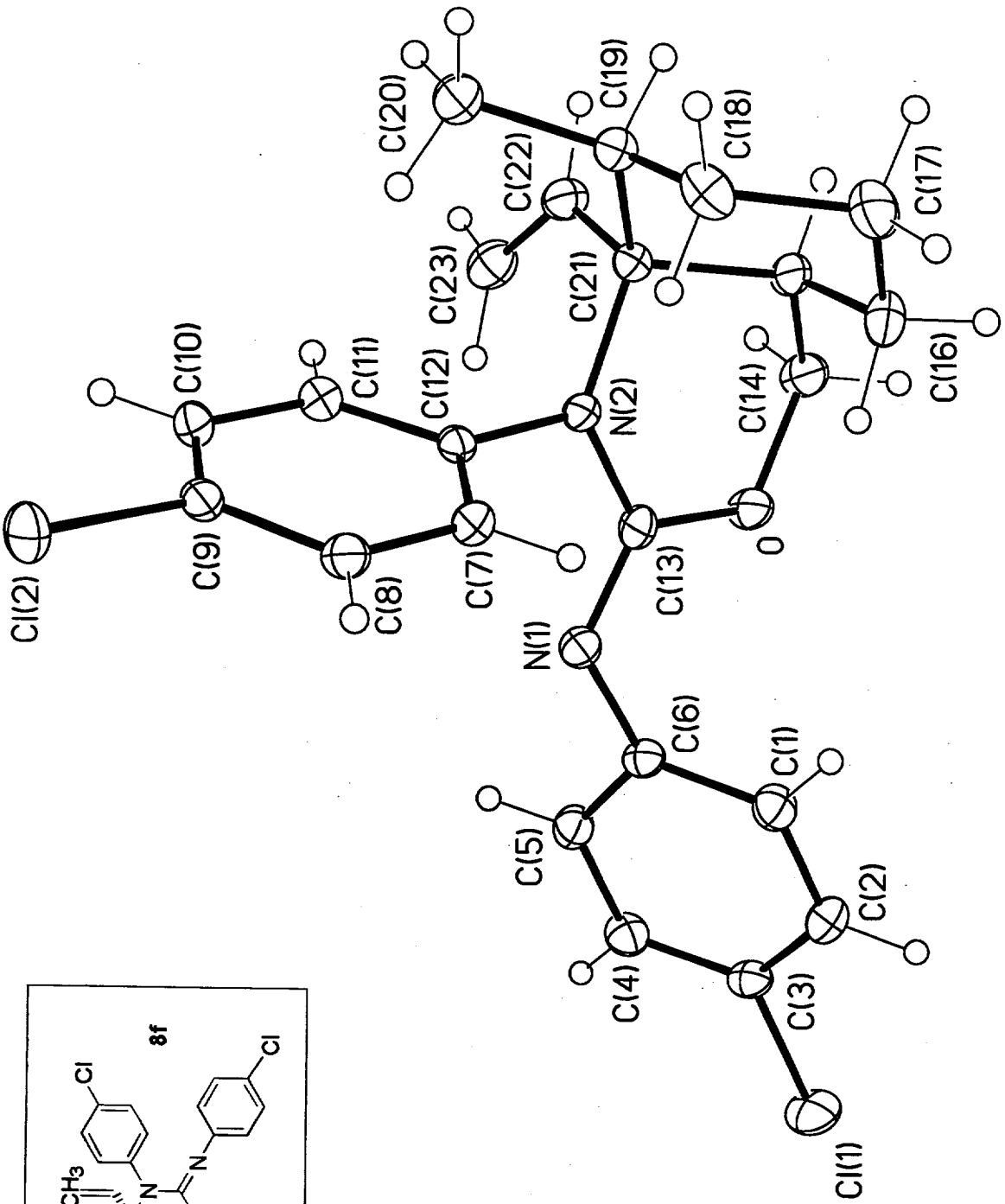

Identification code	ha012
Empirical formula	C23 H24 Cl2 N2 O
Formula weight	415.34
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 7.974(2) A alpha = 104.737(3) deg. b = 9.428(3) A beta = 90.368(4) deg. c = 14.058(4) A gamma = 102.628(4) deg
Volume	995.2(5) A^3
Z, Calculated density	2, 1.386 Mg/m^3
Absorption coefficient	0.343 mm^-1
F(000)	436
Crystal size	0.3 x 0.1 x 0.05 mm
Theta range for data collection	1.50 to 28.60 deg.
Limiting indices	-10<=h<=10, -12<=k<=11, 0<=l<=18
Reflections collected / unique	7931 / 4463 [R(int) = 0.0385]
Completeness to theta = 28.60	87.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4463 / 0 / 253
Goodness-of-fit on F^2	1.006
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1069
R indices (all data)	R1 = 0.0776, wR2 = 0.1122
Largest diff. peak and hole	0.271 and -0.305 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ha012. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cl(1)	1923(1)	1401(1)	6360(1)	50(1)
Cl(2)	4403(1)	2302(1)	-1381(1)	41(1)
N(1)	6080(2)	1968(2)	2938(1)	28(1)
N(2)	8599(2)	2644(2)	2207(1)	27(1)
O	8606(2)	2594(2)	3870(1)	35(1)
C(1)	5273(3)	3047(3)	4601(2)	33(1)
C(2)	4287(3)	2916(3)	5393(2)	34(1)
C(3)	3200(3)	1561(3)	5370(2)	30(1)
C(4)	3080(3)	339(3)	4573(2)	33(1)
C(5)	4061(3)	488(3)	3780(2)	32(1)
C(6)	5190(3)	1841(2)	3782(2)	26(1)
C(7)	6630(3)	3598(3)	1342(2)	28(1)
C(8)	5633(3)	3525(3)	516(2)	29(1)
C(9)	5576(3)	2354(3)	-321(2)	29(1)
C(10)	6422(3)	1245(3)	-325(2)	31(1)
C(11)	7397(3)	1305(3)	511(2)	30(1)
C(12)	7526(3)	2499(2)	1345(1)	24(1)
C(13)	7718(3)	2392(2)	3010(2)	27(1)
C(14)	10463(3)	2871(3)	3936(2)	40(1)
C(15)	11227(3)	3804(3)	3259(2)	35(1)
C(16)	10898(4)	5400(3)	3559(2)	46(1)
C(17)	11637(4)	6348(3)	2877(2)	47(1)
C(18)	10979(3)	5560(3)	1822(2)	41(1)
C(19)	11307(3)	3969(3)	1515(2)	33(1)
C(20)	10991(3)	3326(3)	398(2)	43(1)
C(21)	10512(3)	2953(2)	2190(2)	28(1)
C(22)	11152(3)	1508(3)	1913(2)	35(1)
C(23)	10246(4)	136(3)	1831(2)	41(1)

Table 3. Bond lengths [A] and angles [deg] for ha012.

Cl(1)-C(3)	1.747(2)
Cl(2)-C(9)	1.738(2)
N(1)-C(13)	1.274(3)
N(1)-C(6)	1.404(3)
N(2)-C(13)	1.377(3)
N(2)-C(12)	1.439(2)
N(2)-C(21)	1.490(3)
O-C(13)	1.346(2)
O-C(14)	1.444(3)
C(1)-C(2)	1.383(3)
C(1)-C(6)	1.387(3)
C(2)-C(3)	1.371(3)
C(3)-C(4)	1.373(3)
C(4)-C(5)	1.386(3)
C(5)-C(6)	1.390(3)
C(7)-C(8)	1.381(3)
C(7)-C(12)	1.382(3)
C(8)-C(9)	1.387(3)
C(9)-C(10)	1.362(3)
C(10)-C(11)	1.387(3)
C(11)-C(12)	1.388(3)
C(14)-C(15)	1.501(3)
C(15)-C(16)	1.537(3)
C(15)-C(21)	1.550(3)
C(16)-C(17)	1.510(4)
C(17)-C(18)	1.512(3)
C(18)-C(19)	1.533(3)
C(19)-C(20)	1.529(3)
C(19)-C(21)	1.557(3)
C(21)-C(22)	1.518(3)
C(22)-C(23)	1.313(3)

C(13)-N(1)-C(6)	119.67(18)
C(13)-N(2)-C(12)	114.83(17)
C(13)-N(2)-C(21)	123.78(17)
C(12)-N(2)-C(21)	121.29(17)
C(13)-O-C(14)	121.41(17)
C(2)-C(1)-C(6)	121.7(2)
C(3)-C(2)-C(1)	119.3(2)
C(2)-C(3)-C(4)	120.9(2)
C(2)-C(3)-Cl(1)	119.36(17)
C(4)-C(3)-Cl(1)	119.71(18)
C(3)-C(4)-C(5)	119.3(2)
C(4)-C(5)-C(6)	121.4(2)
C(1)-C(6)-C(5)	117.5(2)
C(1)-C(6)-N(1)	122.9(2)
C(5)-C(6)-N(1)	119.40(19)
C(8)-C(7)-C(12)	120.6(2)
C(7)-C(8)-C(9)	119.2(2)
C(10)-C(9)-C(8)	121.0(2)
C(10)-C(9)-Cl(2)	119.59(17)
C(8)-C(9)-Cl(2)	119.44(19)
C(9)-C(10)-C(11)	119.7(2)
C(10)-C(11)-C(12)	120.2(2)
C(7)-C(12)-C(11)	119.24(19)
C(7)-C(12)-N(2)	118.88(18)

N(1)-C(13)-O	120.4(2)
N(1)-C(13)-N(2)	120.36(18)
O-C(13)-N(2)	119.2(2)
O-C(14)-C(15)	110.92(19)
C(14)-C(15)-C(16)	112.4(2)
C(14)-C(15)-C(21)	108.52(19)
C(16)-C(15)-C(21)	111.97(19)
C(17)-C(16)-C(15)	113.1(2)
C(16)-C(17)-C(18)	110.7(2)
C(17)-C(18)-C(19)	111.3(2)
C(20)-C(19)-C(18)	110.2(2)
C(20)-C(19)-C(21)	118.22(19)
C(18)-C(19)-C(21)	113.78(19)
N(2)-C(21)-C(22)	111.72(18)
N(2)-C(21)-C(15)	106.14(17)
C(22)-C(21)-C(15)	107.57(18)
N(2)-C(21)-C(19)	115.40(18)
C(22)-C(21)-C(19)	108.70(19)
C(15)-C(21)-C(19)	106.88(17)
C(23)-C(22)-C(21)	126.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for ha012.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cl(1)	47(1)	73(1)	35(1)	22(1)	18(1)	14(1)
Cl(2)	40(1)	56(1)	27(1)	10(1)	-7(1)	8(1)
N(1)	28(1)	35(1)	22(1)	12(1)	5(1)	2(1)
N(2)	22(1)	37(1)	19(1)	6(1)	2(1)	6(1)
O	29(1)	57(1)	23(1)	15(1)	3(1)	12(1)
C(1)	34(1)	29(1)	34(1)	9(1)	4(1)	3(1)
C(2)	41(2)	37(2)	26(1)	6(1)	6(1)	11(1)
C(3)	27(1)	43(2)	26(1)	15(1)	5(1)	11(1)
C(4)	32(1)	35(1)	33(1)	14(1)	4(1)	1(1)
C(5)	34(1)	33(1)	27(1)	5(1)	3(1)	5(1)
C(6)	26(1)	34(1)	23(1)	12(1)	4(1)	9(1)
C(7)	28(1)	32(1)	22(1)	5(1)	3(1)	5(1)
C(8)	27(1)	36(1)	28(1)	12(1)	4(1)	10(1)
C(9)	22(1)	40(1)	22(1)	10(1)	1(1)	0(1)
C(10)	28(1)	31(1)	26(1)	1(1)	-1(1)	-2(1)
C(11)	28(1)	31(1)	29(1)	7(1)	2(1)	6(1)
C(12)	19(1)	31(1)	20(1)	8(1)	2(1)	0(1)
C(13)	31(1)	29(1)	19(1)	6(1)	1(1)	8(1)
C(14)	31(1)	68(2)	25(1)	12(1)	-1(1)	18(1)
C(15)	25(1)	56(2)	20(1)	4(1)	-1(1)	11(1)
C(16)	41(2)	53(2)	31(1)	-9(1)	-3(1)	8(1)
C(17)	41(2)	37(2)	52(2)	-2(1)	1(1)	1(1)
C(18)	34(2)	38(2)	47(2)	10(1)	-2(1)	0(1)
C(19)	27(1)	42(2)	28(1)	7(1)	2(1)	4(1)
C(20)	41(2)	55(2)	29(1)	12(1)	4(1)	0(1)
C(21)	22(1)	35(1)	23(1)	5(1)	1(1)	4(1)
C(22)	30(1)	44(2)	34(1)	9(1)	7(1)	11(1)
C(23)	46(2)	43(2)	39(1)	12(1)	7(1)	19(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ha012.

	x	y	z	U(eq)
H(1A)	6019	3977	4619	40
H(2A)	4362	3747	5942	41
H(4A)	2341	-590	4566	40
H(5A)	3962	-342	3228	39
H(7A)	6701	4403	1907	34
H(8A)	5000	4259	522	35
H(10A)	6344	441	-891	37
H(11A)	7972	535	513	36
H(14A)	10813	1908	3762	48
H(14B)	10901	3397	4616	48
H(15A)	12488	3897	3291	41
H(16A)	9653	5327	3568	55
H(16B)	11406	5904	4230	55
H(17A)	12897	6538	2929	57
H(17B)	11312	7321	3073	57
H(18A)	11555	6148	1385	49
H(18B)	9740	5500	1750	49
H(19A)	12567	4124	1637	40
H(20A)	11567	4070	71	65
H(20B)	9764	3073	222	65
H(20C)	11442	2427	195	65
H(22A)	12322	1607	1785	42
H(23C)	9070	-25	1950	49
H(23A)	10774	-685	1654	49