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Crystal structure of 10-(3′-chloropropyl)-2-chlorophenoxazine, $(C_6H_4)ON(C_6H_3)Cl(C_3H_6)Cl$

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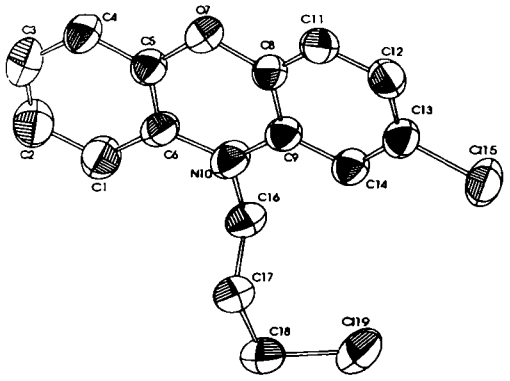

Fig. 1. ORTEP plot of the molecule.

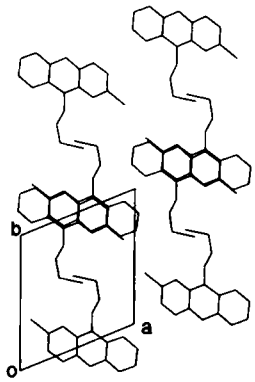

Fig. 2. Packing of the molecules down *c*.

Source of material: synthesized (see ref. 1).
The bond distances and angles do not show any large deviations. The ORTEP plot of the molecule is shown in Fig. 1. Stacking of the molecules is observed when viewed along *c* (Fig. 2).

$C_{15}H_{13}Cl_2NO$, triclinic, $P\bar{1}$ (No. 2), a =9.518(2) Å, b =10.471(2) Å, c =7.865(1) Å, α =100.21(2)°, β =106.26(2)°, γ =65.04(1)°, V =680.6 Å^3, Z =2, $R(F)$ =0.038, $R_w(F^2)$ =0.123.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless, rectangular, size 0.3 x 0.15 x 0.2 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	4.67 cm^{-1}
Diffractometer:	Rigaku AFC7S
Scan mode:	$\omega/2\theta$
$T_{measurement}$:	293 K
$2\theta_{max}$:	50°
$N(hkl)_{unique}$:	2399
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	173
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	2*i*	0.9048(4)	−0.0605(4)	0.1564(5)	0.060(2)	0.056(2)	0.072(2)	−0.019(2)	0.021(2)	0.002(2)
C(2)	2*i*	1.0307(5)	−0.1916(4)	0.1421(5)	0.063(2)	0.069(2)	0.083(3)	−0.018(2)	0.018(2)	0.011(2)
C(3)	2*i*	1.0146(4)	−0.3133(4)	0.1534(5)	0.060(2)	0.057(2)	0.084(3)	−0.004(2)	0.022(2)	0.006(2)
C(4)	2*i*	0.8735(4)	−0.3073(3)	0.1786(5)	0.059(2)	0.040(2)	0.070(2)	−0.009(1)	0.011(2)	0.006(1)
C(5)	2*i*	0.7507(4)	−0.1789(3)	0.1940(4)	0.050(2)	0.043(2)	0.049(2)	−0.015(1)	0.007(1)	0.003(1)
C(6)	2*i*	0.7621(4)	−0.0526(3)	0.1800(4)	0.057(2)	0.038(2)	0.049(2)	−0.016(1)	0.007(1)	0.001(1)
O(7)	2*i*	0.6138(3)	−0.1816(2)	0.2184(3)	0.056(1)	0.040(1)	0.080(2)	−0.016(1)	0.014(1)	−0.002(1)
C(8)	2*i*	0.4948(3)	−0.0542(3)	0.2555(4)	0.046(2)	0.041(2)	0.051(2)	−0.014(1)	0.002(1)	0.004(1)
C(9)	2*i*	0.4996(4)	0.0752(3)	0.2382(4)	0.051(2)	0.039(2)	0.047(2)	−0.016(1)	0.002(1)	0.004(1)

Table 2. (Continued)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(10)	2*i*	0.6287(3)	0.0755(3)	0.1871(4)	0.059(2)	0.039(1)	0.070(2)	−0.018(1)	0.021(1)	0.003(1)
C(11)	2*i*	0.3727(4)	−0.0602(3)	0.3082(4)	0.054(2)	0.047(2)	0.061(2)	−0.022(1)	0.002(1)	0.004(1)
C(12)	2*i*	0.2464(4)	0.0628(4)	0.3426(4)	0.047(2)	0.060(2)	0.058(2)	−0.022(2)	0.007(1)	0.006(1)
C(13)	2*i*	0.2495(4)	0.1895(3)	0.3232(4)	0.050(2)	0.046(2)	0.052(2)	−0.011(1)	0.006(1)	0.003(1)
C(14)	2*i*	0.3737(4)	0.1973(3)	0.2742(4)	0.051(2)	0.042(2)	0.052(2)	−0.016(1)	0.006(1)	0.005(1)
Cl(15)	2*i*	0.0934(1)	0.3469(1)	0.3650(1)	0.0570(6)	0.0573(6)	0.0839(7)	−0.0044(4)	0.0196(4)	0.0033(4)
C(16)	2*i*	0.6286(4)	0.2080(3)	0.1565(4)	0.063(2)	0.038(2)	0.060(2)	−0.021(1)	0.017(2)	0.002(1)
C(17)	2*i*	0.6915(4)	0.2835(3)	0.3239(5)	0.061(2)	0.047(2)	0.071(2)	−0.021(2)	0.012(2)	−0.005(2)
C(18)	2*i*	0.6645(5)	0.4319(4)	0.2935(6)	0.069(2)	0.056(2)	0.105(3)	−0.034(2)	0.025(2)	−0.015(2)
Cl(19)	2*i*	0.4562(1)	0.5419(1)	0.2437(2)	0.0867(7)	0.0448(5)	0.1142(9)	−0.0135(5)	0.0301(6)	−0.0020(5)

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References

1. Sheldrick, G. M.: Phase annealing in SHELX-90: Direct methods for larger structures. Acta Crystallogr. A46 (1990) 467-473.
2. Sheldrick, G. M.: SHELXL-93. Crystal structure refinement program. University of Göttingen, Germany 1993.
3. Thimmaiah, K. N.; Jayashree, B. S.; Horton, J. K.; Germain, G. S.; Dass, C.; Israel, M.; Houghton, P. J.: Synthesis and evaluation of 2-chloro-N^{10}-substituted phenoxazines for circumventing vinblastine resistance in multidrug-resistant cancer cells. J. Med. Chem., submitted.