

**Related literature.** The structure of an analogous ion,  $[\text{TeBr}_{10}]^{2-}$ , has been reported (Krebs & Buscher, 1980). Other dihalogen-bridged structures of selenium that have been determined include  $[\text{SeBr}_6]^{2-}$  (Krebs, Schaffer & Pohl, 1984),  $[\text{Se}_2(\text{CF}_3)_2\text{Cl}_6]$  (Marsden, Sheldrick & Taylor, 1977), and the dimeric  $[\text{SeOCl}_3]^-$  and  $[\text{SeOBr}_3]^-$  ions (Krebs, Schaffer & Hucke, 1982).

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## Structure of [2-(2-Chloroethoxy)ethoxy]-2-methyl-6-morpholinoquinoline\*

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**Abstract.**  $\text{C}_{18}\text{H}_{23}\text{ClN}_2\text{O}_3$ ,  $M_r = 350.8$ , triclinic,  $P\bar{1}$ ,  $a = 6.037$  (1),  $b = 10.208$  (3),  $c = 15.499$  (3) Å,  $\alpha = 103.98$  (2),  $\beta = 82.68$  (2),  $\gamma = 108.56$  (2)°,  $V = 877.4$  (4) Å<sup>3</sup>,  $Z = 2$ ,  $D_m$  (floatation, KI solution) = 1.34,  $D_x = 1.33$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.7107$  Å,  $\mu = 2.41$  cm<sup>-1</sup>,  $F(000) = 372$ ,  $T = 293$  K,  $R = 0.062$  for 882 observed reflections. The morpholine ring adopts a chair conformation while the quinoline ring is planar. The morpholine ring and the side chain are *cis* with respect to the quinoline ring. The sum of the angles around the morpholine N atom is 346.4°.

**Experimental.** The title compound (Fig. 1) was prepared as part of a programme to make compounds with pharmaceutical and insecticidal value. It was prepared by refluxing 6-amino-4-hydroxyquinoline hydrochloride with 2,2'-dichlorodiethyl ether. Crystals were grown from petroleum ether.

Crystal of approximate dimensions 0.18 × 0.25 × 0.58 mm; lattice parameters from 20 reflections (18 <

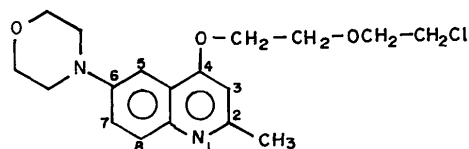


Fig. 1. The title compound.

$2\theta < 34^\circ$ ); intensity data collected on an Enraf-Nonius CAD-4F-11M single-crystal X-ray diffractometer; graphite-monochromated Mo  $K\alpha$  radiation;  $\omega/2\theta$  scan mode; scan speed  $1^\circ \text{ min}^{-1}$ ;  $\theta < 24^\circ$ , index range  $h$  0 to 7,  $k$  -12 to 12,  $l$  -18 to 18; 3040 reflections measured; 882 significant ( $|F_o| > 3\sigma|F_o|$ ). Three standard reflections (00 $\bar{4}$ ,  $\bar{1}\bar{1}\bar{3}$  and  $\bar{1}\bar{3}\bar{7}$ ) measured every 2000 s; 4% variation in intensity; no correction for absorption. Structure solved by direct methods (MULTAN78; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) using a modified procedure (Tavale & Guru Row, 1986); full-matrix refinement of scale factor and non-H-atom positional and anisotropic thermal parameters (positional parameters for H atoms geometrically fixed) converged to  $R = 0.062$  and  $wR =$

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Table 1. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic thermal parameters for non-H atoms with e.s.d.'s in parentheses

$$B_{eq} = \frac{4}{3}(\beta_{11}a^2 + \beta_{22}b^2 + \beta_{33}c^2 + \beta_{12}ab + \beta_{13}ac + \beta_{23}bc).$$

	x	y	z	$B_{eq}(\text{\AA}^2)$
N(1)	3494 (15)	-3505 (7)	4694 (5)	4.42
C(2)	2232 (15)	-2615 (9)	4877 (5)	4.10
C(3)	2579 (16)	-1558 (9)	4394 (6)	4.51
C(4)	4250 (16)	-1390 (9)	3750 (6)	3.95
C(5)	5683 (14)	-2323 (8)	3495 (5)	3.58
C(6)	5184 (15)	-3375 (9)	4016 (5)	3.82
C(7)	6546 (16)	-4302 (9)	3822 (6)	4.39
C(8)	8233 (16)	-4251 (8)	3149 (6)	4.18
C(9)	8665 (15)	-3243 (8)	2610 (6)	3.74
C(10)	7433 (14)	-2265 (8)	2814 (5)	3.55
N(11)	10476 (12)	-3181 (7)	1955 (4)	4.09
Cl	-824 (5)	1206 (4)	1243 (2)	7.81
C(12)	10877 (18)	-2173 (9)	1379 (5)	4.95
C(13)	13145 (19)	-2059 (10)	873 (7)	6.02
O(14)	13392 (11)	-3361 (6)	352 (4)	6.00
C(15)	13096 (20)	-4312 (11)	928 (7)	7.23
C(16)	10765 (18)	-4531 (9)	1426 (6)	5.97
O(17)	4823 (9)	-358 (5)	3256 (3)	4.41
C(18)	3494 (14)	650 (8)	3526 (6)	4.36
C(19)	4511 (15)	1772 (8)	2957 (6)	4.69
O(20)	3437 (10)	1243 (6)	2145 (4)	4.94
C(21)	3734 (19)	2291 (10)	1646 (7)	6.15
C(22)	2185 (16)	1651 (10)	893 (6)	5.40
C(23)	382 (15)	-2797 (9)	5595 (6)	5.10

Table 2. Bond distances ( $\text{\AA}$ ) and bond angles ( $^\circ$ ) with e.s.d.'s in parentheses

N(1)-C(2)	1.32 (1)	C(9)-N(11)	1.39 (1)
N(1)-C(6)	1.37 (1)	N(11)-C(12)	1.47 (1)
C(2)-C(3)	1.41 (1)	N(11)-C(16)	1.47 (1)
C(2)-C(23)	1.47 (1)	Cl-C(22)	1.77 (1)
C(3)-C(4)	1.33 (1)	C(12)-C(13)	1.47 (2)
C(4)-C(5)	1.44 (1)	C(13)-O(14)	1.42 (1)
C(4)-O(17)	1.38 (1)	O(14)-C(15)	1.43 (1)
C(5)-C(6)	1.43 (1)	C(15)-C(16)	1.49 (2)
C(5)-C(10)	1.39 (1)	O(17)-C(18)	1.45 (1)
C(6)-C(7)	1.40 (1)	C(18)-C(19)	1.54 (1)
C(7)-C(8)	1.36 (1)	C(19)-O(20)	1.40 (1)
C(8)-C(9)	1.42 (1)	O(20)-C(21)	1.42 (1)
C(9)-C(10)	1.38 (1)	C(21)-C(22)	1.48 (1)
C(2)-N(1)-C(6)	118.4 (8)	C(6)-C(7)-C(8)	122.1 (9)
N(1)-C(2)-C(3)	121.8 (8)	C(7)-C(8)-C(9)	120.5 (8)
N(1)-C(2)-C(23)	117.4 (8)	C(8)-C(9)-C(10)	118.8 (8)
C(3)-C(2)-C(23)	120.8 (8)	C(8)-C(9)-N(11)	118.7 (8)
C(2)-C(3)-C(4)	120.8 (9)	C(10)-C(9)-N(11)	122.2 (8)
C(3)-C(4)-C(5)	121.2 (9)	C(5)-C(10)-C(9)	120.9 (8)
C(3)-C(4)-O(17)	126.1 (8)	C(9)-N(11)-C(12)	118.8 (7)
C(5)-C(4)-O(17)	112.6 (7)	C(9)-N(11)-C(16)	117.6 (7)
C(4)-C(5)-C(6)	114.0 (7)	C(12)-N(11)-C(16)	109.9 (7)
C(4)-C(5)-C(10)	125.8 (8)	N(11)-C(12)-C(13)	109.9 (8)
C(6)-C(5)-C(10)	120.2 (7)	C(12)-C(13)-O(14)	114.6 (8)
N(1)-C(6)-C(5)	123.8 (8)	C(13)-O(14)-C(15)	108.5 (8)
N(1)-C(6)-C(7)	118.8 (8)	O(14)-C(15)-C(16)	110.9 (9)
C(5)-C(6)-C(7)	117.4 (8)		

0.061,  $S = 2.37$ ,  $w(|F_o| - |F_c|)^2$  minimized where  $w = (10.0 + 1.0|F_o| + 0.014|F_o|^2)^{-1}$ ;  $(\Delta/\sigma)_{\max} = 0.1$ , final  $\Delta\rho$  excursions  $< 10.31 e \text{\AA}^{-3}$ , no correction for secondary extinction, atomic scattering factors from *International Tables for X-ray Crystallography* (1974); the *LALS* program (Gantzel, Sparks & Trueblood,

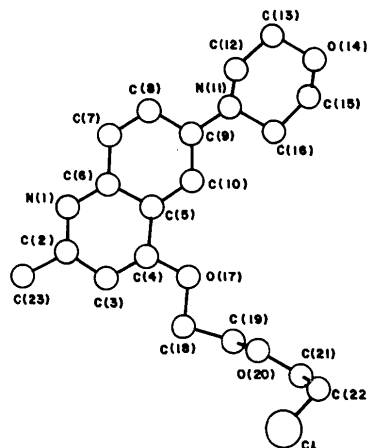


Fig. 2. A perspective view of the molecule along with crystallographic numbering.

1961) was used for refinement. The atomic coordinates with their e.s.d.'s and equivalent isotropic thermal parameters are given in Table 1.\* Bond lengths and bond angles involving the non-H atoms are given in Table 2. Fig. 2 gives a perspective view of the molecule along with the crystallographic numbering of atoms.

**Related literature.** The morpholine ring adopts a chair conformation as is generally found. A survey of known structures involving the morpholine ring (Wong-Ng, Nyburg, Awwal, Jankie & Kresge, 1982) shows the variability in the pyramidity of the bonds attached to the N atom, the sum of the angles around the N atom varying from  $337$  to  $359^\circ$ . In the current example the sum of the angles at N is  $346.4^\circ$ .

\* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44046 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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