Crystal structure of 10-(3'-*N*-morpholinopropyl)-2-trifluoro phenoxazine hydrochloride, C₂₀H₂₁ClF₃N₂O₂

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Fig. 1. ORTEP plot of the molecules.

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

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

Crystal:	transparent, rectangular solid, size 0.1 x 0.2 x 0.2 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	2.40 cm ⁻¹
Diffractometer:	Rigaku AFC7S
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	3467
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	254
Programs:	SHELXS-86, SHELXL-93

Source of material: synthesized (see ref. 1).

The bond distances and angles do not show any large deviations. The thermal ellipsoid plot of the molecule is shown in Fig. 1. The packing of the molecules down *c* is shown in Fig. 2. The molecules are stacked in two layers: one layer has the three fused rings with the fluorine atoms and the other layer has the cyclohexane ring and the free chlorine.

C₂₀H₂₁ClF₃N₂O₂, triclinic, $P\bar{1}$ (No. 2), $a = 9.7757(9)$ Å, $b = 13.826(1)$ Å, $c = 7.4117(9)$ Å, $\alpha = 99.098(9)^\circ$, $\beta = 95.249(9)^\circ$, $\gamma = 89.740(9)^\circ$, $V = 984.9$ Å³, $Z = 2$, $R(F) = 0.090$, $R_w(F^2) = 0.284$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(1)	2i	0.7805(9)	0.7756(6)	-0.210(1)	0.077(5)	0.065(4)	0.058(4)	0.004(4)	0.004(4)	0.004(3)
C(2)	2i	0.8714(9)	0.8128(7)	-0.316(1)	0.060(4)	0.088(6)	0.069(5)	0.006(4)	0.010(4)	-0.002(4)
C(3)	2i	0.831(1)	0.8880(7)	-0.411(1)	0.083(6)	0.084(6)	0.071(5)	-0.017(5)	0.023(4)	0.003(4)
C(4)	2i	0.700(1)	0.9252(6)	-0.399(1)	0.093(6)	0.075(5)	0.051(4)	0.000(4)	0.018(4)	0.016(4)
C(5)	2i	0.6121(8)	0.8888(5)	-0.296(1)	0.080(5)	0.058(4)	0.045(4)	0.004(3)	0.008(3)	0.010(3)

Table 2. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(6)	2i	0.6490(8)	0.8127(5)	−0.1970(9)	0.068(4)	0.049(3)	0.047(3)	0.002(3)	0.006(3)	0.003(3)
O(7)	2i	0.4840(6)	0.9302(4)	−0.2909(8)	0.072(3)	0.086(4)	0.077(4)	0.018(3)	0.021(3)	0.048(3)
C(8)	2i	0.4008(7)	0.9066(5)	−0.1649(9)	0.064(4)	0.055(4)	0.049(4)	0.008(3)	0.006(3)	0.021(3)
C(9)	2i	0.4325(7)	0.8294(5)	−0.0638(9)	0.064(4)	0.044(3)	0.045(3)	0.002(3)	0.001(3)	0.012(3)
N(10)	2i	0.5540(6)	0.7769(4)	−0.0970(9)	0.059(3)	0.058(3)	0.075(4)	0.012(3)	0.009(3)	0.031(3)
C(11)	2i	0.2853(9)	0.9594(6)	−0.143(1)	0.088(5)	0.066(5)	0.063(4)	0.017(4)	0.014(4)	0.031(4)
C(12)	2i	0.1917(8)	0.9380(6)	−0.026(1)	0.064(4)	0.070(5)	0.075(5)	0.027(4)	0.016(4)	0.020(4)
C(13)	2i	0.2188(8)	0.8614(5)	0.073(1)	0.071(4)	0.055(4)	0.055(4)	−0.002(3)	0.007(3)	0.009(3)
C(14)	2i	0.3410(7)	0.8098(5)	0.0552(9)	0.063(4)	0.048(3)	0.051(4)	0.001(3)	0.001(3)	0.014(3)
C(15)	2i	0.119(1)	0.8327(7)	0.195(1)	0.095(6)	0.071(5)	0.077(6)	0.008(5)	0.022(5)	0.017(4)
F(16)	2i	0.0146(7)	0.8926(5)	0.214(1)	0.117(5)	0.113(5)	0.141(6)	0.032(4)	0.074(4)	0.048(4)
F(17)	2i	0.1756(7)	0.8291(7)	0.3618(9)	0.122(5)	0.198(8)	0.078(4)	−0.015(5)	0.028(3)	0.058(4)
F(18)	2i	0.0645(8)	0.7453(5)	0.134(1)	0.140(6)	0.081(4)	0.167(7)	−0.029(4)	0.071(5)	0.011(4)
C(19)	2i	0.5832(7)	0.6940(5)	−0.0004(9)	0.050(3)	0.048(3)	0.059(4)	0.006(3)	−0.005(3)	0.015(3)
C(20)	2i	0.6592(9)	0.7228(5)	0.191(1)	0.084(5)	0.051(4)	0.060(4)	0.003(4)	−0.013(4)	0.005(3)
C(21)	2i	0.6481(8)	0.6451(6)	0.3109(9)	0.069(4)	0.075(5)	0.037(3)	0.009(3)	−0.002(3)	0.008(3)
N(22)	2i	0.7232(6)	0.5518(4)	0.2523(6)	0.073(4)	0.054(3)	0.027(2)	−0.009(2)	0.006(2)	0.011(2)
C(23)	2i	0.6890(8)	0.4773(6)	0.368(1)	0.079(5)	0.086(5)	0.040(3)	−0.015(4)	−0.007(3)	0.031(3)
C(24)	2i	0.773(1)	0.3860(6)	0.326(1)	0.125(8)	0.064(5)	0.061(5)	−0.010(5)	−0.020(5)	0.028(4)
C(26)	2i	0.9482(9)	0.4717(7)	0.232(1)	0.079(5)	0.085(6)	0.055(4)	0.009(4)	−0.015(4)	0.011(4)
C(27)	2i	0.8774(9)	0.5671(6)	0.270(1)	0.094(6)	0.063(4)	0.041(3)	−0.005(4)	0.005(3)	0.014(3)
O(25)	2i	0.9159(7)	0.4066(4)	0.3530(8)	0.101(4)	0.070(3)	0.061(3)	0.014(3)	−0.020(3)	0.022(3)
Cl	2i	0.3142(2)	0.5425(1)	0.1570(2)	0.082(1)	0.058(1)	0.0326(9)	−0.0014(8)	0.0021(7)	0.0085(7)

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