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A monoclinic polymorph of isoxsuprine hydrochloride

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Key indicators

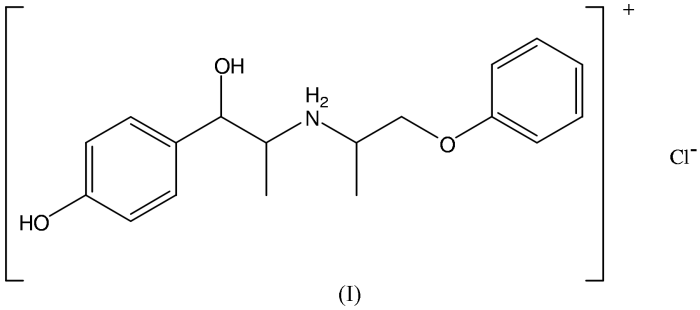
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.095
Data-to-parameter ratio = 17.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

A monoclinic polymorph of the title compound [systematic name: 2-hydroxy-2-(4-methoxyphenyl)-1-methyl-*N*-(1-phenoxy-2-propyl)ethanaminium chloride], $C_{18}H_{24}N_2O_3^+\cdot Cl^-$, has been found in addition to the already known triclinic polymorph. The molecular conformation in both polymorphs is very similar.

Comment

The title compound, (I), is used as a vasodilator and in the treatment of navicular disease. A triclinic polymorph, (II), has already been described (Léger *et al.*, 1981). It crystallizes in $P\overline{1}$ with two molecules in the asymmetric unit. We present here a monoclinic polymorph in $P2_1/c$ with Z = 4. A perspective view of (I) is shown in Fig. 1.



(I)

The cells of the two polymorphs have nothing in common, except the volume. The unit-cell axes and interaxial angles are completely different. The molecular conformations, on the other hand, are essentially the same. A least-squares fit of (I) with (II) gives r.m.s. deviations of 0.228 and 0.200 Å for the two molecules in the asymmetric unit of (II) (Fig. 2).

The crystal packing is stabilized by several N—H···Cl and O—H···Cl hydrogen bonds (Table 1).

Experimental

The sample of the title compound was obtained as a gift from Jayco Chemical Industries, India. It was used without further purification and recrystallized from methanol.

Crystal data

$C_{18}H_{24}NO_3^+\cdot Cl^-$
M_r = 337.83
Monoclinic, $P2_1/c$
a = 12.0767 (11) Å
b = 19.3499 (12) Å
c = 7.8018 (7) Å
β = 107.482 (7)°
V = 1738.9 (3) Å^3
Z = 4
D_x = 1.290 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 065 reflections
θ = 3.7–27.6°
μ = 0.23 mm^{-1}
T = 173 (2) K
Block, colourless
0.44 × 0.39 × 0.35 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.904, T_{max} = 0.923
21 164 measured reflections
4008 independent reflections
3499 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.7°
$h = -15 \rightarrow 15$
$k = -25 \rightarrow 25$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.095
S = 1.07
4008 reflections
224 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.1915P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···Cl1^{i}	0.78 (2)	2.36 (2)	3.1285 (11)	168.3 (18)
N3—H3A···Cl1^{ii}	0.895 (16)	2.529 (16)	3.3726 (10)	157.2 (13)
N3—H3B···Cl1	0.844 (17)	2.344 (17)	3.1852 (11)	174.3 (14)
O14—H14···Cl1^{iii}	0.84 (3)	2.33 (3)	3.1730 (11)	178 (2)

Symmetry codes: (i) $x, y, z-1$; (ii) $x, \frac{1}{2}-y, z-\frac{1}{2}$; (iii) $1-x, 1-y, 1-z$.

H atoms bonded to carbon were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl})] using a riding model, with C—H = 1.00, 0.99, 0.98 and 0.95 Å for tertiary CH, secondary CH, methyl and aromatic CH, respectively. H atoms bonded to nitrogen and oxygen were refined freely.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

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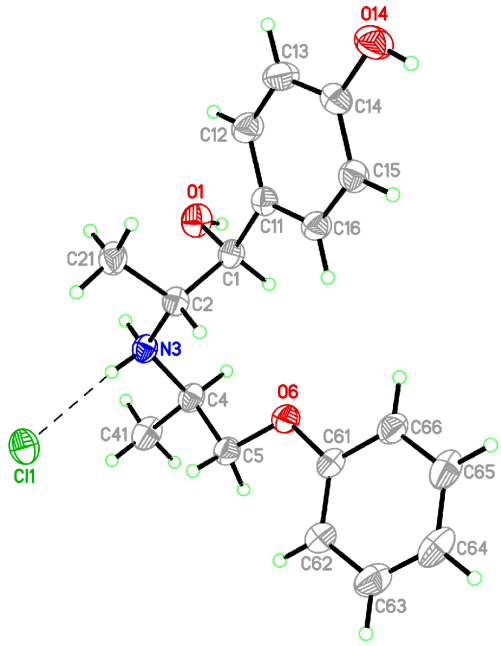

Figure 1
Perspective view of the title compound with the atom numbering; displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a hydrogen bond.

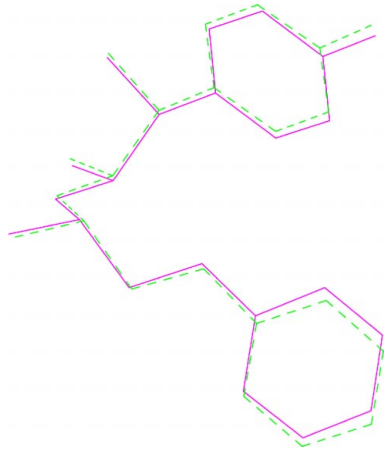

Figure 2
Least-squares fit of (I) (dashed line) with one of the two molecules (solid line) in the asymmetric unit of (II).

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