Structure of *R*-(1-Naphtyl)ethylamine Hydrochloride Monohydrate

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The title compound (Fig. 1), *R*-NPEA, is one of the useful resolving agents of chiral acids. The degree of chiral discrimination and the efficiency of the optical agents are considered to be dependent on the three-dimensional structures of the agents. In order to understand the mechanism of chiral recognition of *R*-NPEA, the inherent three-dimensional structure of this useful optical selector was determined by X-ray analysis.

The gelation of a chloroform solution of *R*-NPEA (1% v/v) takes place by diffusing hydrogen chloride into the solution. The gel was dissolved in ethanol and colorless rod-like crystals were obtained from the solution at 297(2)K. A crystal with dimensions of $0.30 \times 0.20 \times 0.20$ mm was used for diffraction experiments. The crystal and experimental data are given in Table 1. The structure was solved by direct methods and

Fig. 1 Chemical structure.

Table 1 Crystal and experimental data

Formula: C ₁₂ H ₁₆ NOCl
Formula weight = 225.72
Crystal system: monoclinic
Space group: <i>P</i> 2 ₁ <i>Z</i> = 2
<i>a</i> = 10.6050(7) Å
<i>b</i> = 7.3924(4) Å β = 103.495(5)°
<i>c</i> = 8.0816(4) Å
<i>V</i> = 616.08(6) Å ³
<i>D</i> _x = 1.217 Mg m ⁻³
No. of reflections used = 2644
2θ _{max} = 148° with Cu Kα
<i>R</i> = 0.041
(Δ/ <i>σ</i>) _{max} = 0.05
(Δρ) _{max} = 0.43
(Δρ) _{min} = -0.28
Measurement: Enraf-Nonius CAD-4 Turbo
Program system: Rigaku teXsan ¹
Structure determination: SIR88 ²
Refinement: full-matrix

refined with anisotropic temperature factors for non-H atoms. All H atoms were found from difference Fourier maps. The H atoms were refined with isotropic temperature factors. The absolute configuration, determined using anomalous dispersion by chlorine, confirms the *R* configuration. The atomic parameters for non-hydrogen atoms are listed in Table 2.

An ORTEP II³ drawing of the title compound together with the atomic numbering is shown in Fig. 2. The bond distances and angles are tabulated in Table 3. The two phenyl rings are essentially planar. The dihedral angles between the mean planes is 2.82(7)° and the naphthyl ring is significantly folded across the central C-C bond toward the C2 atom. The ethyl group is almost perpendicular to the naphthyl ring with the torsion angles of C2-C1-C3-C10a and N1-C1-C3-C4 being 79.3(2) and 24.0(2)°, respectively. The C6a-C10a bond is significantly longer than other bonds in the naphthyl ring. The shortest bond in the ring is the C5-C6 bond. The C6a-C10a-C10 and C6a-C10a-C3 bond angles are significantly smaller than the others inside the naphthyl ring. The exocyclic bond angles around the C3 atom are highly asymmetrical. *R*-NPEA molecules, chloride ions and water molecules form an extensive hydrogen bond network in the crystal. *R*-NPEA molecules are connected through chloride ions and water molecules. There are four intermolecular hydrogen bonds [O-H...Cl = 3.257(2), ∠O-H...Cl = 168(4)°; O-H...Cl (2-*x*,

Table 2 Atomic coordinates and equivalent isotropic thermal parameters (*B*_{eq})

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq}
C1	0.00573(4)	0	0.74582(6)	3.330(9)
O	0.0456(2)	0.1765(3)	1.1475(2)	4.06(4)
N	0.0881(2)	0.4748(3)	0.6589(2)	2.73(3)
C1	0.2290(2)	0.5248(2)	0.7188(2)	2.42(3)
C2	0.2493(2)	0.7090(3)	0.6462(3)	3.10(4)
C3	0.3154(2)	0.3793(2)	0.6716(2)	2.33(3)
C4	0.2702(2)	0.2635(3)	0.5384(2)	2.91(4)
C5	0.3510(2)	0.1291(3)	0.4928(3)	3.45(4)
C6	0.4759(2)	0.1137(3)	0.5805(3)	3.29(4)
C6a	0.5287(2)	0.2334(3)	0.7153(2)	2.62(3)
C7	0.6614(2)	0.2254(3)	0.8007(3)	3.29(4)
C8	0.7132(2)	0.3447(4)	0.9267(3)	3.60(4)
C9	0.6337(2)	0.4764(4)	0.9772(3)	3.66(4)
C10	0.5047(2)	0.4868(3)	0.8984(2)	3.05(4)
C10a	0.4477(2)	0.3686(2)	0.7635(2)	2.35(3)

$$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}(a_i\cdot a_j).$$

Fig. 2 ORTEP drawing of the molecule, representing heavy atoms as 50% probability ellipsoids and H atoms as spheres of arbitrary radius.

$1/2+y, 1-z = 3.172(2)$, $\angle \text{O-H}\cdots\text{Cl} = 157(3)^\circ$; $\text{N-H}\cdots\text{Cl} = 3.186(2)$, $\angle \text{N-H}\cdots\text{Cl} = 165(3)^\circ$; $\text{N-H}\cdots\text{Cl} (2-x, 1/2+y, 2-z) = 3.279(2)$, $\angle \text{N-H}\cdots\text{Cl} = 173(3)^\circ$.

References

1. teXsan, "Single Crystal Structure Analysis Software,"

Table 3 Bond distances (Å) and angles (°)

N	---	C1	1.506(2)	C1	---	C2	1.518(3)				
C1	---	C3	1.518(2)	C1	---	C2	1.518(3)				
C3	---	C10a	1.429(2)	C4	---	C5	1.415(3)				
C5	---	C6	1.354(3)	C6	---	C6a	1.414(3)				
C6a	---	C7	1.417(3)	C6a	---	C10a	1.431(2)				
C7	---	C8	1.362(4)	C8	---	C9	1.410(4)				
C9	---	C10	1.370(3)	C10	---	C10a	1.417(3)				
N	---	C1	---	C2	108.4(1)	N	---	C1	---	C3	110.9(1)
C2	---	C1	---	C3	113.0(1)	C1	---	C3	---	C4	121.3(2)
C1	---	C3	---	C10a	119.0(2)	C4	---	C3	---	C10a	119.6(2)
C3	---	C4	---	C5	121.4(2)	C4	---	C5	---	C6	120.0(2)
C5	---	C6	---	C6a	120.9(2)	C6	---	C6a	---	C7	121.2(2)
C6	---	C6a	---	C10a	119.5(2)	C7	---	C6a	---	C10a	119.2(2)
C6a	---	C7	---	C8	121.2(2)	C7	---	C8	---	C9	120.0(2)
C8	---	C9	---	C10	120.3(2)	C9	---	C10	---	C10a	121.5(2)
C3	---	C10a	---	C6a	118.5(2)	C3	---	C10a	---	C10	123.8(2)
C6a	---	C10a	---	C10	117.7(2)						

Version 1.6", 1993, Molecular Structure Corporation, Texas, U.S.A.

2. M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, G. Polidori, R. Spagna, and D. Voterbo, *J. Appl. Cryst.*, **1989**, 22, 389.
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