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Key indicators

Single-crystal X-ray study

T = 298 K

Mean $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$

R factor = 0.077

wR factor = 0.241

Data-to-parameter ratio = 15.4

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.4-Chloro-2-[[*(R)*-(3'*S*,8'*R*)-3,3*a*,8,8*a*-tetrahydro-2*H*-indeno[1,2-*d*][1,3]oxazol-3-yl)](phenyl)methyl]-phenol

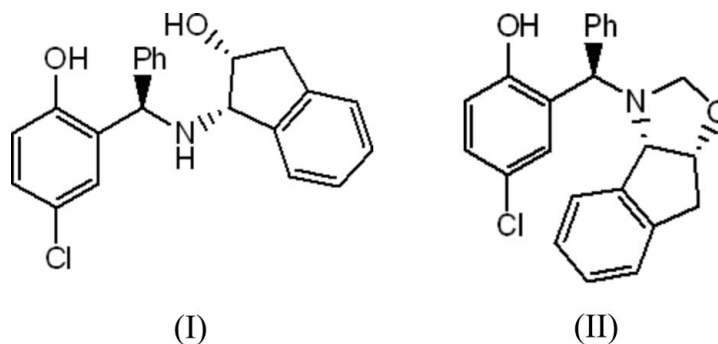
The asymmetric unit contains two independent molecules of the title compound, $\text{C}_{23}\text{H}_{20}\text{ClNO}_2$, with the same absolute configuration. Intramolecular O—H···N hydrogen bonding is observed in both independent molecules.

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Comment

Chiral aminophenols have attracted increasing attention because of their possible application in asymmetric catalytic reactions (Cimarelli *et al.*, 2001). Recently, we prepared a new chiral amino phenol, (I), by a condensation reaction of (1*S*,2*R*)-1-amino-2-indanol and (5-chloro-2-hydroxyphenyl)-(phenyl)methanone followed by reduction with NaBH_4 . The above reaction generated a new chiral center at the C atom attached to the phenol group. The title compound, (II), has been prepared by the reaction of (I) with formaldehyde. We obtained single crystals of (II) and have determined the structure of (II), leading to the determination of the absolute configuration at the new chiral center in (I).



The asymmetric unit of (II) contains two molecules (Fig. 1), with the same absolute configuration of 1*S*,2*R*,1'*R*. The configuration at the new chiral centers (C11 and C30) is unambiguously determined to be *R*. Thus, we infer that the absolute configuration for (I) is also 1*S*,2*R*,1'*R*. In both molecules, the bond distances are normal. Intramolecular O—H···N hydrogen bonds, which help to stabilize the molecular structure, are observed in both independent molecules of (II) (Table 1).

Experimental

Compound (I) was reacted with formaldehyde (1.2 equivalents) in a methanol solution (10 ml) at room temperature to obtain (II). The detailed procedure is similar to that reported by Yang *et al.* (2005). After solvent had been removed under reduced pressure, the solid product was recrystallized from an ethyl acetate/ethanol solution (90:1 v/v) to obtain single crystals of (II).

Crystal data

C₂₃H₂₀CINO₂M_r = 377.85Orthorhombic, P2₁2₁2₁

a = 9.5270 (12) Å

b = 18.657 (2) Å

c = 22.679 (3) Å

V = 4031.2 (9) Å³

Z = 8

D_x = 1.245 Mg m⁻³

Mo Kα radiation

μ = 0.21 mm⁻¹

T = 298 (2) K

Block, colorless

0.60 × 0.54 × 0.45 mm

Data collection

Bruker SMART CCD area-detector
diffractometer

φ and ω scans

Absorption correction: none

21356 measured reflections

7508 independent reflections
4295 reflections with I > 2σ(I)R_{int} = 0.041θ_{max} = 25.5°

Refinement

Refinement on F²R[F² > 2σ(F²)] = 0.077wR(F²) = 0.241

S = 1.00

7508 reflections

487 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.1469P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ (Δ/σ)_{max} = 0.002Δρ_{max} = 0.57 e Å⁻³Δρ_{min} = -0.42 e Å⁻³

Absolute structure: Flack (1983),

3287 Friedel pairs

Flack parameter: 0.03 (13)

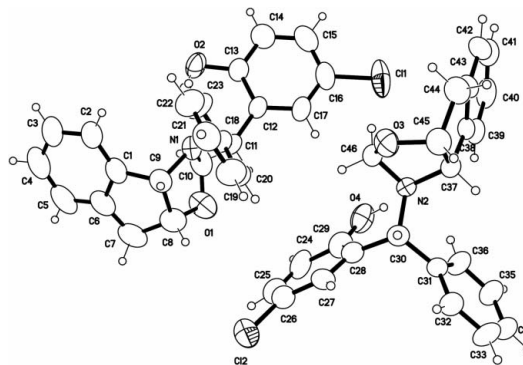


Figure 1

The asymmetric unit of (II), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Table 1

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
O2—H2...N1	0.82	1.94	2.636 (5)	142
O4—H4...N2	0.82	2.03	2.709 (6)	140

H atoms were placed in calculated positions, with C—H = 0.93 (aromatic), 0.97 (methylene) or 0.98 Å (methine) and O—H = 0.82 Å, and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}(O)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine

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