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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.037
 wR factor = 0.125
Data-to-parameter ratio = 8.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

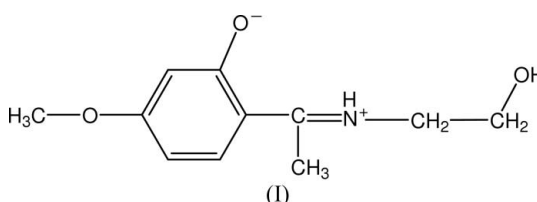
2-[1-(2-Hydroxyethyliminio)ethyl]-5-methoxyphenolate

The title Schiff base compound, $\text{C}_{11}\text{H}_{15}\text{NO}_3$, synthesized by the reaction of paeonol and ethanolamine in absolute methanol, crystallizes in a zwitterionic form. All non-H atoms except the hydroxyl O atom are approximately coplanar. Molecules are linked by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds into chains along the [100] direction.

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Comment

Paeonol, 2-hydroxyl-4-methoxyacetophenone, is an effective component of traditional Chinese medicines, and its derivatives have attracted considerable attention because of their potential biological activities. Many new metallic complexes of paeonol have been prepared and characterized; however, structural studies of them have rarely been reported (Sillanpaa, 1991; Demertzi *et al.*, 2000). As part of our ongoing investigation on Schiff base compounds of paeonol (Xu *et al.*, 2006), we present here the structure of the title compound, (I).



The molecular structure of (I) is shown in Fig. 1. The molecule is in a zwitterionic form with a strong intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond (Table 1). The $\text{C}-\text{C}$ bond distances in the benzene ring lie in the range 1.359 (3)–1.434 (3) Å and the $\text{C}-\text{C}-\text{C}$ bond angles vary from 118.0 (2) to 122.5 (2)°. The $\text{C}7-\text{N}1$ bond distance of 1.302 (3) Å is typical for a $\text{C}=\text{N}$ double bond. The $\text{C}-\text{O}^-$ bond distance [1.291 (3) Å] is shorter than the value of 1.326 Å reported in the literature (Li *et al.*, 2003; Zhou & Duan, 1995). This may be due to the effect of hyperconjugation. Atoms C10 and O2 deviate from the mean plane formed by the rest of the non-H atoms in the molecule by 1.061 (2) and -0.151 (2) Å, respectively.

Molecules of the title compound are linked by $\text{O}-\text{H}\cdots\text{O}$ (Table 1, Fig. 2) hydrogen bonds into chains along the [100] direction.

Experimental

To a stirred absolute methanol solution (25 ml) of paeonol (0.83 g, 5 mmol) was added dropwise an absolute methanol solution (10 ml) of ethanolamine (0.31 g, 5.0 mmol) at room temperature. After stirring for 3 h at 320 K, the precipitate was filtered off, washed with

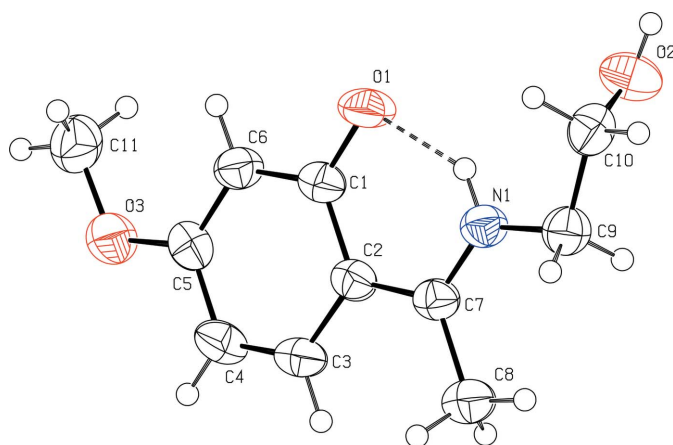


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids.

methanol and dried *in vacuo*. Single crystals of (I) were obtained by slow evaporation of the resulting filtrate after 4 d (m.p. 422.8–423.4 K). Analysis found: C 63.25, H 7.14, N 6.70%; calculated for $C_{11}H_{15}NO_3$: C 63.17, H 7.18, N 6.71%.

Crystal data

$C_{11}H_{15}NO_3$	$Z = 4$
$M_r = 209.24$	$D_x = 1.315 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 6.2552 (5) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$b = 6.3403 (5) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 26.648 (2) \text{ \AA}$	Block, yellow
$V = 1056.86 (15) \text{ \AA}^3$	$0.35 \times 0.32 \times 0.30 \text{ mm}$

Data collection

Bruker APEX area-detector diffractometer	5346 measured reflections
φ and ω scans	1133 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2002)	1061 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.967$, $T_{\max} = 0.972$	$R_{\text{int}} = 0.019$
	$\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1088P)^2 + 0.0099P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.126$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
1133 reflections	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
136 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2-H2A\cdots O1^i$	0.82	1.91	2.708 (2)	164
$N1-H1\cdots O1$	0.86	1.80	2.533 (3)	141

Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{5}{2}, -z + 2$.

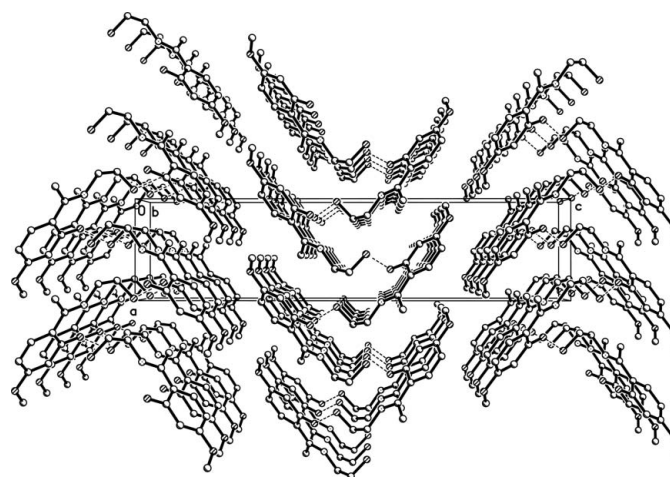


Figure 2
The crystal packing of (I), viewed down the b axis. Dashed lines indicate hydrogen bonds.

The H atom on the imino N atom was located in a difference map and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. Other H atoms were positioned geometrically with $O-H = 0.82 \text{ \AA}$, $C-H = 0.93$ (aromatic), 0.96 (methyl) or 0.97 \AA (methylene), and refined in riding mode with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C/O})$ for methyl and hydroxyl H atoms or $1.2U_{\text{eq}}(\text{C})$ for other atoms. A rotating group model was used for the methyl groups. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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