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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 = 0.054
 wR factor = 0.132
 Data-to-parameter ratio = 13.9

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

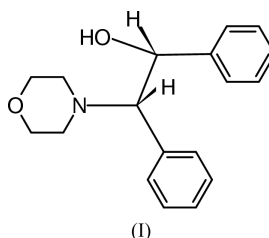
erythro-2-Morpholino-1,2-diphenylethanol

The title compound, $\text{C}_{18}\text{H}_{21}\text{NO}_2$, consists of two aromatic rings and a morpholine ring attached to an ethanol moiety. The molecule is non-planar. There is an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond.

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Comment

Photo-initiated free-radical polymerization is of great commercial importance (Davidson, 1999; Pappas, 1978). Techniques such as curing of the coating on various materials, adhesives, printing inks, and photoresists are based on photo-initiated free-radical polymerization. The title compound, (I), was synthesized and used for the polymerization of acrylates and methacrylates (Davidson & Steiner, 1971; Arsu & Aydın, 1999). In this paper we report the structure of (I).



The molecular structure of (I) is shown in Fig. 1. The C5—C12 distance of 1.563 (3) Å is nearly equal to the value of 1.520 (3) Å in (*E,E*)-4-[3-(dichloro-2-hydroxyphenylazo)-2-morpholino-2-butenoyl]morpholine (Ramm *et al.*, 1995). The N1—C1 and N1—C4 bond lengths are 1.472 (3) and 1.475 (3) Å, respectively, and agree with the corresponding distances in 1,3-bis(2-methylphenyl)-2-(4-morpholino)isothiourea [1.473 (3) and 1.470 (4) Å; Sudha *et al.*, 1996]. The N1—C5 and C12—O2 bond lengths are 1.491 (2) and 1.441 (3) Å, respectively; these are similar to the corresponding bond lengths in the salt of diclofenac with *N*-(2-hydroxyethyl)morpholine [1.489 (4) and 1.403 (4) Å, respectively; Castellari & Sabatino, 1996]. There is an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond (Table 2). The crystal structure is stabilized by van der Waals interactions.

The molecule (I) contains three ring systems, two phenyl rings and a morpholino ring. For the morpholine ring we calculated, following the method of Cremer & Pople (1975), a phase angle $\theta_2 = 0.030$ (2)° and $\varphi_2 = 320$ (5)°, indicating a chair conformation, and a puckering amplitude $Q = 0.580$ (2) Å.

Experimental

trans-Stilbene oxide (1 g) and 1 molar equivalent of distilled morpholine was refluxed for 12 h with vigorous stirring. The product was extracted with diethyl ether and the excess of morpholine were

separated by addition of 5 ml of distilled water. The combined organic layers were washed with distilled water several times. The solution was dried over anhydrous magnesium sulfate. The crude product of (I) was recrystallized from ethanol. Analysis calculated for $C_{18}H_{21}NO_2$: C 76.30, H 7.54, N 5.01%; analysis found: C 76.43, H 7.60, N 4.93; m.p. 394 K. 1H NMR (100 MHz) in $CDCl_3$: δ 7.08–7.30 (*m*, 10H), 4.89 (*m*, 1H), 3.89 (*m*, 1H), 3.43 (*m*, 4H), 3.35 (*s*, 1H), 2.61 (*m*, 4H).

Crystal data

$C_{18}H_{21}NO_2$	$D_x = 1.192 \text{ Mg m}^{-3}$
$M_r = 283.36$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3846 reflections
$a = 13.4628 (7) \text{ \AA}$	$\theta = 3.1\text{--}28.3^\circ$
$b = 5.8074 (3) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 20.3321 (11) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 96.611 (10)^\circ$	Slab, colourless
$V = 1579.07 (14) \text{ \AA}^3$	$0.36 \times 0.30 \times 0.16 \text{ mm}$
$Z = 4$	

Data collection

Siemens SMART CCD area-detector diffractometer	1426 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.082$
Absorption correction: none	$\theta_{\text{max}} = 25.0^\circ$
6883 measured reflections	$h = -16 \rightarrow 14$
2711 independent reflections	$k = -6 \rightarrow 6$
	$l = -22 \rightarrow 24$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2)]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$wR(F^2) = 0.132$	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
$S = 0.73$	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$
2711 reflections	Extinction correction: <i>SHELXL</i>
195 parameters	Extinction coefficient: 0.044 (4)
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters (\AA , $^\circ$).

N1—C1	1.472 (3)	C1—C2	1.514 (3)
N1—C4	1.475 (3)	C3—C4	1.517 (3)
N1—C5	1.491 (2)	C5—C6	1.525 (3)
O1—C2	1.421 (3)	C5—C12	1.563 (3)
O1—C3	1.424 (3)	C12—C13	1.515 (3)
O2—C12	1.441 (3)		
C1—N1—C4	107.14 (18)	N1—C4—C3	110.67 (19)
C1—N1—C5	113.11 (15)	N1—C5—C6	111.92 (16)
C4—N1—C5	112.15 (16)	N1—C5—C12	108.37 (15)
C2—O1—C3	109.36 (18)	C6—C5—C12	111.00 (17)
N1—C1—C2	110.11 (18)	C7—C6—C5	122.58 (19)
O1—C2—C1	111.5 (2)	O2—C12—C5	109.85 (16)
O1—C3—C4	112.3 (2)	C13—C12—C5	113.02 (16)

Table 2

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O2-H2A \cdots N1$	0.89 (3)	2.31 (3)	2.821 (2)	116 (2)

The hydroxy-H atom was located from a difference Fourier map and refined isotropically. The other H atoms were positioned geometrically and refined using a riding model.

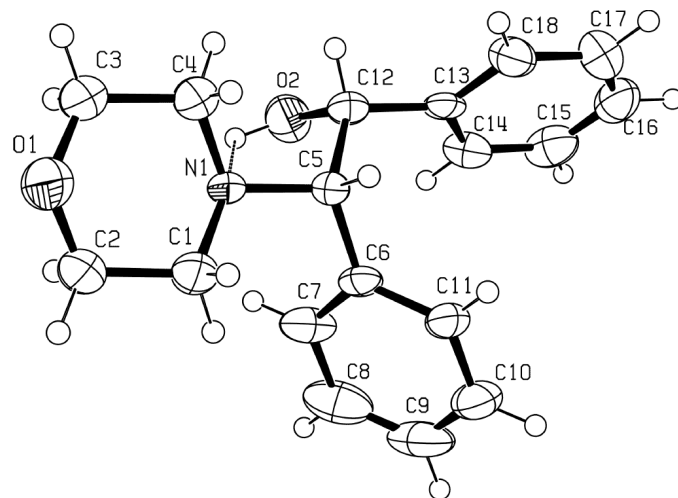


Figure 1

An ORTEPIII drawing (Burnett & Johnson, 1996) of (I), showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are shown at the 50% probability level.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 1997).

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