

**(E)-1-(2-Hydroxyphenyl)propan-2-one  
O-methoxime forms hydrogen-  
bonded chains of edge-fused  $R_4^4(16)$   
and  $R_4^4(24)$  rings**Christopher Glidewell,<sup>a\*</sup> John N. Low,<sup>b</sup>  
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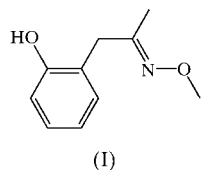
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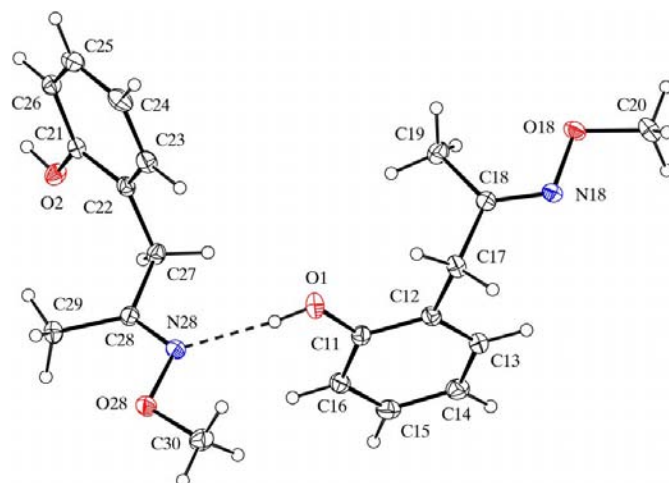
The title compound,  $C_{10}H_{13}NO_2$ , crystallizes with  $Z' = 2$  in space group  $P\bar{1}$ . The molecules are linked by two  $O-H\cdots N$  hydrogen bonds [ $H\cdots O = 1.97$  and  $1.98$  Å,  $O\cdots N = 2.810$  (2) and  $2.815$  (2) Å, and  $O-H\cdots N = 175$  and  $174^\circ$ ] and by one  $C-H\cdots O$  hydrogen bond [ $H\cdots O = 2.50$  Å,  $C\cdots O = 3.313$  (2) Å and  $C-H\cdots O = 144^\circ$ ] into chains of edge-fused centrosymmetric rings in which  $R_4^4(16)$  and  $R_4^4(24)$  rings alternate.

**Comment**

The title compound, (I), was originally prepared as part of a study of the cyclization reactions of phenolic oximes (Forrester *et al.*, 1975). Its structure has now been determined in order to establish both the geometry at the oxime group and the nature of the supramolecular interactions.



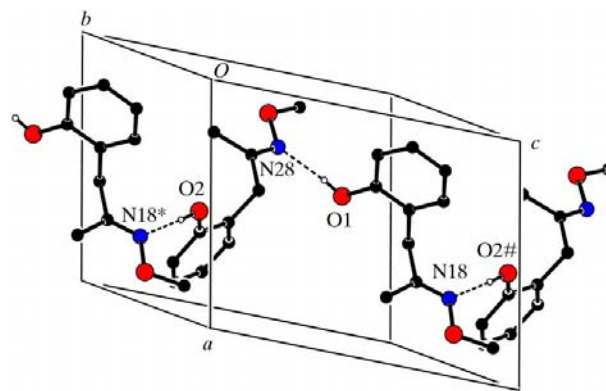
Compound (I) crystallizes in space group  $P\bar{1}$ , with two independent molecules in the asymmetric unit (Fig. 1). Both molecules have the *E* configuration at the  $C=N$  bond. The intramolecular dimensions are very similar in the two molecules, and the bond distances show no unusual features. The angles at the planar C atoms C18 and C28 show considerable variation from  $120^\circ$  (Table 1) and both of the  $C-N-O$  angles are substantially less than  $120^\circ$ . As shown by the leading torsion angles, the conformations of the two molecules are very similar.

**Figure 1**

The two independent molecules in compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

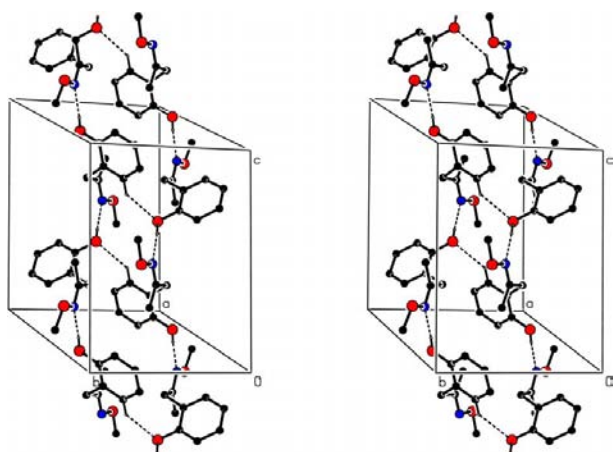
The molecules of (I) are linked into a chain of edge-fused rings by the combination of two nearly linear  $O-H\cdots N$  hydrogen bonds and one rather weak  $C-H\cdots O$  hydrogen bond (Table 2). Within the asymmetric unit, phenolic atom O1 in the type 1 molecule (containing O1, *etc.*) acts as hydrogen-bond donor to oxime atom N28 in the type 2 molecule (containing O2, *etc.*) (Fig. 1), and in a similar way, phenolic atom O2 in the type 2 molecule at  $(x, y, z)$  acts as hydrogen-bond donor to oxime atom N18 in the type 1 molecule at  $(x, y, z - 1)$ . The combination of these two hydrogen bonds then generates by translation a  $C_2^2(14)$  (Bernstein *et al.*, 1995) chain running parallel to the  $[001]$  direction (Fig. 2).

Two such chains, related to one another by inversion, pass through each unit cell, and these two chains are weakly linked by the  $C-H\cdots O$  hydrogen bond. Aryl atom C23 in the type 2 molecule at  $(x, y, z)$  acts as hydrogen-bond donor to phenolic atom O1 in the type 1 molecule at  $(1 - x, 1 - y, 1 - z)$ , so

**Figure 2**

Part of the crystal structure of (I), showing the formation of a  $C_2^2(14)$  chain along  $[001]$ . For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (\*) or a hash (#) are at the symmetry positions  $(x, y, z - 1)$  and  $(x, y, 1 + z)$ , respectively.

generating by inversion an  $R_4^4(16)$  ring centred at  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . Propagation by translation and inversion of the  $R_4^4(16)$  motif linking antiparallel  $C_2^2(14)$  chains then generates an [001] chain of edge-fused rings, with  $R_4^4(16)$  rings centred at  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} + n)$  ( $n = \text{zero or integer}$ ) alternating with  $R_4^4(24)$  rings centred at  $(\frac{1}{2}, \frac{1}{2}, n)$  ( $n = \text{zero or integer}$ ) (Fig. 3).



**Figure 3**

A stereoview of part of the crystal structure of (I), showing the formation of a chain of alternating and edge-fused  $R_4^4(16)$  and  $R_4^4(24)$  rings. For the sake of clarity, H atoms bonded to C atoms have been omitted.

There are no direction-specific interactions between adjacent chains of rings in (I). In particular, there are neither C—H... $\pi$ (arene) hydrogen bonds nor aromatic  $\pi$ — $\pi$  stacking interactions present in the structure.

## Experimental

The title compound, (I), was prepared (Forrester *et al.*, 1975) from 2-hydroxyphenylpropanone (Tinsley, 1959) and *O*-methylhydroxylamine. Crystals of (I) suitable for single-crystal X-ray diffraction were grown by slow evaporation of a solution in ethanol (m.p. 350–352 K).

### Crystal data

$C_{10}H_{13}NO_2$	$Z = 4$
$M_r = 179.21$	$D_x = 1.211 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 9.3723$ (2) Å	Cell parameters from 4492 reflections
$b = 9.4254$ (2) Å	reflections
$c = 12.3080$ (3) Å	$\theta = 3.0$ – $27.6^\circ$
$\alpha = 89.7146$ (12) $^\circ$	$\mu = 0.09 \text{ mm}^{-1}$
$\beta = 68.5508$ (11) $^\circ$	$T = 120$ (2) K
$\gamma = 77.0903$ (10) $^\circ$	Plate, colourless
$V = 982.85$ (4) Å $^3$	$0.20 \times 0.20 \times 0.04 \text{ mm}$

### Data collection

Nonius KappaCCD area-detector diffractometer	4492 independent reflections
$\varphi$ scans, and $\omega$ scans with $\kappa$ offsets	3441 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SORTAV; Blessing, 1995, 1997)	$R_{\text{int}} = 0.033$
$T_{\text{min}} = 0.978$ , $T_{\text{max}} = 0.997$	$\theta_{\text{max}} = 27.6^\circ$
8474 measured reflections	$h = -12 \rightarrow 12$
	$k = -12 \rightarrow 12$
	$l = -15 \rightarrow 15$

### Refinement

Refinement on $F^2$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.051$	$\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$
$wR(F^2) = 0.154$	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
$S = 1.09$	Extinction correction: SHELXL97 (Sheldrick, 1997)
4492 reflections	Extinction coefficient: 0.034 (6)
240 parameters	
H-atom parameters constrained	
$w = 1/[\sigma^2(F_o^2) + (0.0707P)^2 + 0.2766P]$	
where $P = (F_o^2 + 2F_c^2)/3$	

**Table 1**

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

O1—C11	1.367 (2)	O2—C21	1.368 (2)
C18—N18	1.278 (2)	C28—N28	1.280 (2)
N18—O18	1.422 (2)	N28—O28	1.420 (2)
C17—C18—N18	116.52 (14)	C27—C28—N28	115.95 (13)
C17—C18—C19	118.82 (14)	C27—C28—C29	119.00 (14)
N18—C18—C19	124.62 (15)	N28—C28—C29	125.01 (15)
C18—N18—O18	111.66 (13)	C28—N28—O28	112.21 (12)
N18—O18—C20	108.27 (12)	N28—O28—C30	107.86 (12)
C11—C12—C17—C18	−117.67 (16)	C21—C22—C27—C28	−109.88 (16)
C17—C18—N18—O18	178.57 (12)	C27—C28—N28—O28	179.05 (12)
C18—N18—O18—C20	−171.79 (13)	C28—N28—O28—C30	179.96 (14)
C19—C18—N18—O18	1.0 (2)	C29—C28—N28—O28	1.4 (2)

**Table 2**

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1...N28	0.84	1.98	2.815 (2)	174
O2—H2...N18 <sup>i</sup>	0.84	1.97	2.810 (2)	175
C23—H23...O1 <sup>ii</sup>	0.95	2.50	3.313 (2)	144

Symmetry codes: (i)  $x, y, z - 1$ ; (ii)  $1 - x, 1 - y, 1 - z$ .

Crystals of compound (I) are triclinic; space group  $P\bar{1}$  was selected and confirmed by the successful structure analysis. All H atoms were located from difference maps and subsequently treated as riding atoms, with C—H distances of 0.95 (aromatic), 0.98 (CH<sub>3</sub>) or 0.99 Å (CH<sub>2</sub>), and O—H distances of 0.84 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{O})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

Data collection: KappaCCD Server Software (Nonius, 1997); cell refinement: DENZO-SMN (Otwinowski & Minor, 1997); data reduction: DENZO-SMN; program(s) used to solve structure: OSCAIL (McArdle, 2003) and SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: OSCAIL and SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97 and PRPKAPPA (Ferguson, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1704). Services for accessing these data are described at the back of the journal.

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