

Table 2. Selected geometric parameters (Å, °)

N1—C2	1.47 (1)	C16—O17	1.36 (1)
N1—C9A	1.37 (1)	O17—C18	1.383 (7)
N1—C10	1.477 (7)	C18—C19	1.34 (1)
C2—C3	1.509 (9)	C1'—C2'	1.40 (1)
C2—C11	1.52 (1)	C1'—C6'	1.395 (9)
C3—N4	1.460 (6)	C2'—C12'	1.710 (7)
N4—C5	1.311 (9)	C2'—C3'	1.379 (8)
C5—C5A	1.42 (1)	C3'—C4'	1.36 (1)
C5—C1'	1.498 (7)	C4'—C14'	1.719 (7)
C5A—C6	1.43 (1)	C4'—C5'	1.37 (1)
C5A—C9A	1.444 (7)	C5'—C6'	1.394 (9)
C6—C7	1.36 (1)	C1''—C2''	1.38 (1)
C7—C8	1.420 (7)	C1''—C6''	1.39 (1)
C8—O8	1.37 (1)	C1''—S7''	1.771 (9)
C8—C9	1.37 (1)	C2''—C3''	1.37 (1)
O8—C8M	1.440 (7)	C3''—C4''	1.39 (1)
C9—C9A	1.42 (1)	C4''—C4''M	1.51 (1)
C11—N12	1.44 (1)	C4''—C5''	1.37 (2)
N12—C13	1.347 (6)	C5''—C6''	1.36 (1)
C13—O14	1.220 (9)	S7''—O8''	1.447 (5)
C13—C15	1.47 (1)	S7''—O9''	1.45 (1)
C15—C16	1.36 (1)	S7''—O10''	1.444 (4)
C15—C19	1.441 (8)		
C9A—N1—C10	119.2 (7)	C15—C16—O17	110.1 (6)
C2—N1—C10	112.2 (7)	C16—O17—C18	106.9 (7)
C2—N1—C9A	127.3 (5)	O17—C18—C19	110.2 (7)
N1—C2—C11	111.3 (5)	C15—C19—C18	106.7 (6)
N1—C2—C3	112.4 (7)	C5—C1'—C6'	120.8 (6)
C3—C2—C11	113.3 (6)	C5—C1'—C2'	121.0 (6)
C2—C3—N4	111.7 (5)	C2'—C1'—C6'	118.1 (6)
C3—N4—C5	122.0 (6)	C1'—C2'—C3'	122.1 (6)
N4—C5—C1'	114.2 (6)	C1'—C2'—C12'	120.5 (6)
N4—C5—C5A	124.6 (6)	C12'—C2'—C3'	117.4 (5)
C5A—C5—C1'	121.2 (7)	C2'—C3'—C4'	118.4 (6)
C5—C5A—C9A	126.5 (8)	C3'—C4'—C5'	121.8 (7)
C5—C5A—C6	115.3 (6)	C3'—C4'—C14'	119.9 (6)
C6—C5A—C9A	118.1 (7)	C14'—C4'—C5'	118.4 (6)
C5A—C6—C7	123.6 (6)	C4'—C5'—C6'	120.1 (7)
C6—C7—C8	116.4 (9)	C1'—C6'—C5'	119.6 (7)
C7—C8—C9	123.2 (7)	C6'—C1''—S7''	121.2 (8)
C7—C8—O8	113.6 (7)	C2''—C1''—S7''	120.0 (7)
O8—C8—C9	123.1 (6)	C2''—C1''—C6''	118.8 (8)
C8—O8—C8M	117.6 (8)	C1''—C2''—C3''	120
C8—C9—C9A	120.8 (6)	C2''—C3''—C4''	121 (1)
C5A—C9A—C9	117.7 (7)	C3''—C4''—C5''	118 (1)
N1—C9A—C9	116.7 (6)	C3''—C4''—C4''M	120 (1)
N1—C9A—C5A	125.5 (8)	C4''M—C4''—C5''	122 (1)
C2—C11—N12	112.7 (6)	C4''—C5''—C6''	122 (1)
C11—N12—C13	118.7 (6)	C1''—C6''—C5''	120 (1)
N12—C13—C15	116.9 (6)	C1''—S7''—O10''	106.3 (3)
N12—C13—O14	121.9 (8)	C1''—S7''—O9''	105.5 (4)
O14—C13—C15	121.2 (6)	C1''—S7''—O8''	106.7 (3)
C13—C15—C19	125.3 (6)	O9''—S7''—O10''	112.3 (3)
C13—C15—C16	128.5 (7)	O8''—S7''—O10''	112.7 (3)
C16—C15—C19	106.1 (7)	O8''—S7''—O9''	112.7 (4)
C2—N1—C9A—C5A	26 (1)	N4—C5—C1'—C6'	-58 (1)
C9A—N1—C2—C11	-112.5 (9)	N4—C5—C5A—C9A	-31 (1)
C9A—N1—C2—C3	16 (1)	C5—C5A—C9A—N1	-1 (1)
N1—C2—C11—N12	-158.1 (6)	C2—C11—N12—C13	83.3 (9)
N1—C2—C3—N4	-74.3 (8)	C11—N12—C13—O14	-7 (1)
C2—C3—N4—C5	69.4 (9)	C11—N12—C13—C15	170.4 (7)
C3—N4—C5—C5A	-2 (1)	N12—C13—C15—C19	-177.8 (8)

Data collection was performed with a fixed scan width and a 2:1 ratio of peak-counting time to background-counting time. The structure was solved by direct methods and refined by full-matrix least squares. H-atom positions were calculated where possible; others were obtained from a difference Fourier synthesis. The largest density of 0.91 e Å<sup>-3</sup> in the final difference Fourier map is near the H6' position, suggesting some partial occupancy of C12' (180° rotational disorder of the 2,4-dichlorophenyl ring). Data collection and cell refinement: Hilger & Watts Y290 software. Data reduction: REDU4 (Stoe

& Cie, 1992). Program(s) used to solve structure: MULTAN80 (Main *et al.*, 1980). Program(s) used to refine structure: NRCVAX (Gabe, Le Page, Charland, Lee & White, 1989). Molecular graphics: PLUTO (Motherwell & Clegg, 1978). Software used to prepare material for publication: PARST (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1088). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## 4-Hydroxyacetophenone Oxime (I) and 4-Hydroxy-3-methylacetophenone Oxime (II)

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## Abstract

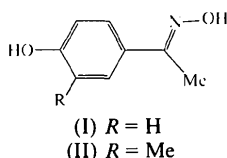
The crystal structures of the two chemically similar compounds (I), C<sub>8</sub>H<sub>9</sub>NO<sub>2</sub>, and (II), C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>, have been determined at room temperature. Despite the

close relationship between the molecular structures, significantly different hydrogen-bonding schemes were observed in the crystal structures of (I) and (II).

### Comment

As a continuation of investigations of compounds capable of forming polar chains of molecules, several oximes containing a second functional group have been studied (Padmanabhan, Paul & Curtin, 1989; Maurin, Paul & Curtin, 1992, 1994; Maurin, Wieteska & Winnicka-Maurin, 1994). This paper presents two hydroxyoxime structures. For some time the complexing and extracting properties of aliphatic and aromatic hydroxyoximes have been used in industry for the hydrometallurgical recovery of copper, nickel, germanium and rare metals such as palladium, molybdenum and vanadium (Szymanowski, 1993). Hydroxyoximes form chelate complexes where the oxime and hydroxyl groups are coordinated by metal ions while the remaining part of the hydroxyoximes form hydrophobic envelopes around the metal.

The conformation and packing of the molecules and the numbering of the atoms are shown in Figs. 1 and 2 for (I) and (II), respectively.



Crystals of (II) show the commonly observed centrosymmetric oxime-oxime dimer structure. On the other hand, the previously reported infinite polar chains of molecules may also be observed. They are approximately parallel to the *c* direction (Padmanabhan, Paul & Curtin, 1989; Maurin, Paul & Curtin, 1992, 1994). It should be pointed out that there is a difference in chain formation. In 'carboxyl-oxime' structures the chains are composed of pairs of hydrogen bonds, namely, carboxyl-oxime  $O-H \cdots N$  and oxime-carboxyl  $O-H \cdots O$ , whereas the chains in the structure of (II) are formed by only one hydroxyl-oxime hydrogen bond,  $O-H \cdots O$ .

The structure of 4-hydroxyacetophenone oxime (I) is more complex; a cyclic tetramer is combined with a chain feature. The structure shows some resemblance to the structures of levulinic acid oxime and 4-methyl-2-oxopentanoic acid oxime (Maurin, Leś & Winnicka-Maurin, 1994), in which cyclic tetramers were also observed. Two types of hydrogen bonds are present in the structure of (I), namely, oxime-hydroxyl  $O-H \cdots O$  and hydroxyl-oxime  $O-H \cdots N$ . Anti-parallel polar chains of the form oxime-hydroxyl-oxime-hydroxyl, parallel to the *b* axis, are bonded together by hydroxyl-oxime  $O-H \cdots N$  hydrogen bonds. A comparison of the hydrogen bonds geometries is given in Table 5.

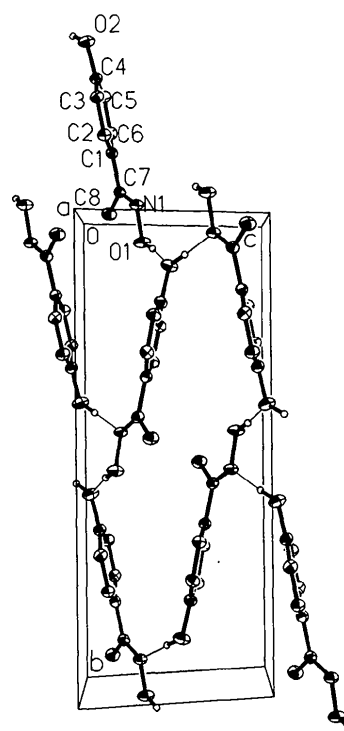


Fig. 1. View of the crystal structure of 4-hydroxyacetophenone oxime with the atomic numbering. The hydrogen bonds are marked as thin lines. Displacement ellipsoids are plotted at the 50% probability level.

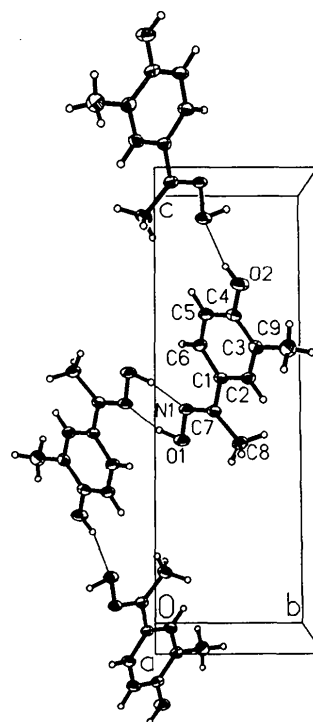


Fig. 2. View of the crystal structure of 4-hydroxy-3-methylacetophenone oxime with the atomic numbering. The hydrogen bonds are marked as thin lines. Displacement ellipsoids are plotted at the 50% probability level.

## Experimental

4-Hydroxyacetophenone oxime (I) and 4-hydroxy-3-methylacetophenone oxime (II) were obtained by the reaction of hydroxylamine hydrochloride in alkaline solution with 4-hydroxyacetophenone and 4-hydroxy-3-methylacetophenone, respectively. The products were both recrystallized from ethanol–water solution. Crystals of (I) suitable for X-ray measurements were obtained from benzene–ethanol solution (m.p. 420–421 K), and those of (II) were obtained from ethanol–water solution (m.p. 425 K).

## Compound (I)

## Crystal data

C<sub>8</sub>H<sub>9</sub>NO<sub>2</sub>  
*M<sub>r</sub>* = 151.16  
 Monoclinic  
*P*2<sub>1</sub>/*n*  
*a* = 6.6640 (10) Å  
*b* = 16.830 (4) Å  
*c* = 7.153 (2) Å  
 $\beta$  = 107.898 (6)°  
*V* = 763.4 (3) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.315 Mg m<sup>-3</sup>

Mo *K*α radiation  
 $\lambda$  = 0.71073 Å  
 Cell parameters from 17 reflections  
 $\theta$  = 4.8–9.8°  
 $\mu$  = 0.095 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Transparent columnar  
 0.7 × 0.5 × 0.2 mm  
 Colourless

## Data collection

Syntex *P*2<sub>1</sub> four-circle diffractometer  
 Separate  $\omega/2\theta$  scans  
 Absorption correction: none  
 1527 measured reflections  
 1184 independent reflections  
 987 observed reflections  
 [*I* > 2σ(*I*)]

*R*<sub>int</sub> = 0.029  
 $\theta_{\max}$  = 25.00°  
 $h = -7 \rightarrow 7$   
 $k = 0 \rightarrow 20$   
 $l = 0 \rightarrow 8$   
 3 standard reflections monitored every 200 reflections  
 intensity variation: none

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.0374  
 $\omega R(F^2) = 0.0902$   
*S* = 1.114  
 1184 reflections  
 144 parameters  
 All H-atom parameters refined  
 Calculated weights  
 $w = 1/[\sigma^2(F_o^2) + (0.0257P)^2 + 0.1561P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

( $\Delta/\sigma$ )<sub>max</sub> = -0.003  
 $\Delta\rho_{\max} = 0.114 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.160 \text{ e } \text{Å}^{-3}$   
 Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>) for (I)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>eq</sub>
C1	-0.0377 (2)	-0.15911 (10)	0.1550 (2)	0.0430 (4)
C2	0.1410 (3)	-0.19103 (11)	0.1217 (3)	0.0485 (5)
C3	0.1532 (3)	-0.27103 (11)	0.0825 (3)	0.0505 (5)
C4	-0.0147 (3)	-0.32050 (10)	0.0734 (3)	0.0485 (5)
C5	-0.1919 (3)	-0.29077 (11)	0.1095 (3)	0.0524 (5)
C6	-0.2038 (3)	-0.21038 (11)	0.1470 (3)	0.0492 (5)
C7	-0.0502 (3)	-0.07343 (10)	0.1989 (3)	0.0459 (4)
C8	-0.2554 (3)	-0.03062 (14)	0.1300 (4)	0.0610 (6)

N1	0.1236 (2)	-0.03972 (8)	0.2953 (2)	0.0498 (4)
O1	0.0997 (2)	0.04223 (7)	0.3239 (2)	0.0655 (4)
O2	0.0002 (2)	-0.39926 (8)	0.0248 (2)	0.0662 (5)

Table 2. Selected geometric parameters (Å, °) for (I)

C1—C6	1.391 (2)	C4—O2	1.382 (2)
C1—C2	1.392 (2)	C5—C6	1.386 (3)
C1—C7	1.484 (2)	C7—N1	1.283 (2)
C2—C3	1.383 (3)	C7—C8	1.489 (3)
C3—C4	1.380 (3)	N1—O1	1.411 (2)
C4—C5	1.378 (3)		
C6—C1—C2	117.8 (2)	C3—C4—O2	118.1 (2)
C6—C1—C7	121.1 (2)	C4—C5—C6	119.6 (2)
C2—C1—C7	121.2 (2)	C5—C6—C1	121.4 (2)
C3—C2—C1	121.1 (2)	N1—C7—C1	116.32 (15)
C4—C3—C2	120.0 (2)	N1—C7—C8	123.3 (2)
C5—C4—C3	120.1 (2)	C1—C7—C8	120.4 (2)
C5—C4—O2	121.8 (2)	C7—N1—O1	112.77 (14)

## Compound (II)

## Crystal data

C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>  
*M<sub>r</sub>* = 165.19  
 Monoclinic  
*P*2<sub>1</sub>/*n*  
*a* = 10.273 (2) Å  
*b* = 5.3870 (10) Å  
*c* = 15.843 (3) Å  
 $\beta$  = 97.035 (5)°  
*V* = 870.2 (3) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.261 Mg m<sup>-3</sup>

Mo *K*α radiation  
 $\lambda$  = 0.71073 Å  
 Cell parameters from 20 reflections  
 $\theta$  = 4.8–10.4°  
 $\mu$  = 0.090 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Transparent prismatic  
 0.5 × 0.3 × 0.3 mm  
 Colourless

## Data collection

Syntex *P*2<sub>1</sub> four-circle diffractometer  
 Separate  $\omega/2\theta$  scans  
 Absorption correction: none  
 1861 measured reflections  
 1233 independent reflections  
 930 observed reflections  
 [*I* > 2σ(*I*)]

*R*<sub>int</sub> = 0.116  
 $\theta_{\max}$  = 25.00°  
 $h = -12 \rightarrow 12$   
 $k = 0 \rightarrow 6$   
 $l = 0 \rightarrow 18$   
 3 standard reflections monitored every 200 reflections  
 intensity variation: none

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.0732  
 $\omega R(F^2) = 0.2033$   
*S* = 1.161  
 1233 reflections  
 125 parameters  
 Only H-atom *U*'s refined  
 Calculated weights  
 $w = 1/[\sigma^2(F_o^2) + (0.1373P)^2 + 0.5164P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

( $\Delta/\sigma$ )<sub>max</sub> = 0.001  
 $\Delta\rho_{\max} = 0.248 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.242 \text{ e } \text{Å}^{-3}$   
 Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 3. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>) for (II)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>eq</sub>
O1	0.0029 (3)	0.1812 (5)	0.42030 (14)	0.0661 (8)
N1	0.0981 (3)	0.2087 (5)	0.49354 (15)	0.0561 (8)
O2	0.5625 (3)	0.5486 (6)	0.7694 (2)	0.0782 (10)

C1	0.2729 (3)	0.4366 (6)	0.5650 (2)	0.0506 (8)
C2	0.3708 (3)	0.6132 (7)	0.5642 (2)	0.0577 (9)
C3	0.4664 (3)	0.6578 (7)	0.6318 (2)	0.0574 (9)
C4	0.4651 (3)	0.5107 (7)	0.7043 (2)	0.0574 (9)
C5	0.3671 (4)	0.3358 (7)	0.7083 (2)	0.0644 (10)
C6	0.2726 (4)	0.2998 (7)	0.6398 (2)	0.0611 (10)
C7	0.1738 (3)	0.3958 (7)	0.4898 (2)	0.0539 (9)
C8	0.1638 (4)	0.5693 (8)	0.4155 (2)	0.0709 (12)
C9	0.5682 (4)	0.8561 (9)	0.6283 (3)	0.0799 (13)

Table 4. Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ) for (II)

O1—N1	1.431 (3)	C2—C3	1.382 (5)
N1—C7	1.279 (5)	C3—C4	1.397 (5)
O2—C4	1.362 (4)	C3—C9	1.501 (5)
C1—C2	1.386 (5)	C4—C5	1.386 (5)
C1—C6	1.396 (5)	C5—C6	1.379 (5)
C1—C7	1.486 (4)	C7—C8	1.497 (5)
C7—N1—O1	113.8 (3)	O2—C4—C5	122.5 (3)
C2—C1—C6	116.6 (3)	O2—C4—C3	117.3 (3)
C2—C1—C7	121.4 (3)	C5—C4—C3	120.2 (3)
C6—C1—C7	122.0 (3)	C6—C5—C4	120.4 (3)
C3—C2—C1	124.0 (3)	C5—C6—C1	121.3 (3)
C2—C3—C4	117.5 (3)	N1—C7—C1	116.1 (3)
C2—C3—C9	121.8 (3)	N1—C7—C8	123.0 (3)
C4—C3—C9	120.7 (3)	C1—C7—C8	120.8 (3)

Table 5. Comparison of hydrogen-bonding geometries ( $\text{\AA}$ ,  $^\circ$ ) of the two title structures

$D-H \cdots A$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
Compound (I)			
O1—HO1 $\cdots$ O2 <sup>i</sup>	1.82 (3)	2.734 (2)	174 (2)
O2—HO2 $\cdots$ N1 <sup>ii</sup>	1.74 (3)	2.742 (2)	176 (2)
Compound (II)			
O1—HO1 $\cdots$ N1 <sup>iii</sup>	1.75 (4)	2.774 (4)	165 (3)
O2—HO2 $\cdots$ O1 <sup>iv</sup>	1.99 (5)	2.825 (4)	165 (4)

Symmetry codes: (i)  $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$ ; (ii)  $-\frac{1}{2} + x, -\frac{1}{2} - y, -\frac{1}{2} + z$ ; (iii)  $-x, -y, 1 - z$ ; (iv)  $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$ .

All the H atoms in structure (I), including those of the disordered methyl group, were located from the  $\Delta\rho$  map. In structure (II), oxime and hydroxyl H atoms were found in a  $\Delta\rho$  map, while all other H atoms were included in their calculated positions. In the final cycle of refinement of (I), refinement was carried out on the positions of all atoms, with anisotropic displacement parameters for non-H atoms and isotropic displacement coefficients for ordered H atoms. For the disordered H atoms the relative site occupancy [0.60 (2) for atoms *a*, *b* and *c* attached to C8] and a common isotropic displacement parameter were refined. In structure (II), the non-H atoms were refined with anisotropic displacement parameters. Oxime and hydroxyl H-atom positions, the individual isotropic displacement parameters for the benzene-type H atoms, common isotropic displacement parameters and relative site occupancies for disordered methyl H atoms [0.54 (4) for atoms *a*, *b* and *c* attached to C8 and C9] were refined.

There was some trouble with the data collection for (II), caused by the quality of crystals obtained. This, in turn, resulted in a paucity of data and the high values of  $R_{\text{int}}$  and  $R$  but there were no problems in solving and refining the structure.

*SHELXS86* (Sheldrick, 1990) was used for structure solution; refinement was performed using *SHELXL* (Sheldrick, 1994). Molecular graphics were prepared using *ORTEP* (Johnson, 1976). The material for publication was produced using *SHELXL93*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1131). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## 2'-Hydroxypropiophenone Oxime

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## Abstract

The title structure,  $\text{C}_9\text{H}_{11}\text{NO}_2$ , consists of antiparallel polar chains of molecules, bonded together by a series of intra- and intermolecular hydrogen bonds between oxime and hydroxyl groups. None of the usual oxime–oxime hydrogen bonds has been observed.

## Comment

As a continuation of studies of oxime molecules with a second functional group, possessing donor–acceptor capabilities (Maurin, Paul & Curtin, 1992, 1994; Maurin, Winnicka-Maurin & Leś, 1994), several hydroxy–oxime structures have been determined (Maurin, 1994; Maurin, Wieteska & Winnicka-Maurin, 1994). 2'-Hydroxypropiophenone oxime, (I), is the first hydroxy–oxime structure in which intra- and intermolecular hydrogen bonds are combined in a chain formation. The conformation of the molecules and the numbering of the atoms are given in Fig. 1. The hydrogen-