pyrone moiety. In this context, we have already determined several structures of flavones (Wallet, Gaydou, Fadlane & Baldy, 1988; Wallet, Gaydou & Baldy, 1989). The observed bond lengths are similar to the values reported for 5,6-benzoflavone (Rossi, Cantrell, Farber, Dyott, Carrell & Glusker, 1980) and 5-hydroxy-6,7,8,3′,4′,5′-hexamethoxyflavone (Vijayalakshmi, Rajan & Srinivasan, 1987), particularly the C2—C1′ bond linking the phenyl ring and the γ-benzopyrone moiety at 1·460 (5) and 1·468 (5) Å respectively.

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Structure of Racemic 4-Isopropenyl-1-cyclohexene-1-carbaldehyde Oxime (Perillartine)

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Abstract. $C_{10}H_{15}NO$, $M_r = 165{\cdot}23$, triclinic, $P\bar{1}$, $a = 7{\cdot}3217\,(6)$, $b = 8{\cdot}1899\,(6)$, $c = 8{\cdot}8402\,(8)$ Å, $\alpha = 104{\cdot}551\,(1)$, $\beta = 96{\cdot}215\,(7)$, $\gamma = 104{\cdot}591\,(1)°$, $V = 488{\cdot}14\,(7)$ Å^3, $Z = 2$, $D_x = 1{\cdot}124$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71073$ Å, $\mu = 0{\cdot}7$ cm^{-1}, $F(000) = 180$, $T = 298$ K, $R = 0{\cdot}049$ for 1275 unique observed diffractometer data $[I \geq 2{\cdot}5\sigma(I)]$. A partial substitutional disorder of enantiomers was observed. The molecules form O—H···N-type cyclic hydrogen-bonded dimers across inversion centers. A systematic search for the so-called *A*H—*B* moieties which are thought to be responsible for the sweet taste revealed a CH—O moiety with a C···O distance of 2·22 Å as the only candidate.

Experimental. The title compound has an intensely sweet taste (Beets, 1978; van der Heijden, van der Wel & Peer, 1985) and a structure determination was undertaken to elucidate the molecular conformation in order to identify the origin of the sweet taste in terms of the so-called *A*H—*B* moiety (Shallenberger & Acree, 1967).

The title compound was recrystallized by sitting-drop vapor diffusion (McPherson, 1976) using 2-propanol as solvent and water as precipitant. Two sets of data were collected (November 1985 and August 1989) on a CAD-4F diffractometer at ambient temperature for two transparent, colorless crystals (0·2 × 0·3 × 0·3 mm, 0·4 × 0·2 × 0·2 mm), mounted on a glass fiber. Collection of data set 1: 876 reflections were scanned [h: -8, 0; $h = 2n$; k: -9, 9; l: -10, 10; $\theta \leq 24{\cdot}99°$; $\omega/2\theta$-scan mode; $\Delta\omega = (0{\cdot}60 + 0{\cdot}35\tan\theta)°$; Zr-filtered Mo $K\alpha$ radiation]. During the measurement three reference reflections ($\bar{2}00$, 010, 002) showed fluctuations of 3%, and negligible decay during 35 h of X-ray exposure time. The data were corrected for Lp but not for absorption. $\sigma^2(I) = \sigma^2_{\rm cs}(I) + (pI)^2$ (McCandlish, Stout & Andrews, 1975) with $p = 0{\cdot}02$. Collection of data set 2: 3243 reflections were scanned [h: -9, 0; k: -10, 10; l: -11, 11; $\theta \leq 28{\cdot}47°$; $\omega/2\theta$-scan mode; $\Delta\omega = (0{\cdot}65 + 0{\cdot}35\tan\theta)°$; Zr-filtered Mo $K\alpha$ radiation]. During the measurement three reference reflections (012, $\bar{2}04$, $\bar{3}30$) showed fluctuations of 4%, and a decay of about 20% during the 43 h of X-ray exposure time, for which a linear correction was

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Table 1. *Final coordinates and equivalent isotropic thermal parameters with e.s.d.'s in parentheses for the molecule with higher occupation factor*

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

	x	y	z	U_{eq}(Å^2)
O	0·1234 (3)	0·2077 (2)	0·0870 (2)	0·0871 (6)
N	0·1935 (2)	0·0683 (2)	0·1086 (2)	0·0702 (6)
C(1)	0·4651 (3)	0·0015 (2)	0·2195 (2)	0·0627 (6)
C(2)	0·6476 (3)	0·0599 (2)	0·2900 (2)	0·0742 (7)
C(3)	0·7647 (3)	−0·0528 (2)	0·3327 (2)	0·0771 (7)
C(4)	0·6665 (4)	−0·2474 (3)	0·2505 (5)	0·064 (1)
C(5)	0·4580 (4)	−0·2911 (3)	0·2607 (5)	0·075 (1)
C(6)	0·3552 (3)	−0·1898 (2)	0·1770 (3)	0·0806 (8)
C(7)	0·3669 (3)	0·1234 (3)	0·1814 (2)	0·0693 (7)
C(8)	0·7761 (6)	−0·3634 (5)	0·3030 (6)	0·064 (1)
C(9)	0·8702 (8)	−0·4445 (8)	0·2083 (8)	0·084 (2)
C(10)	0·7826 (9)	−0·3857 (8)	0·4709 (9)	0·103 (2)

applied. The data were corrected for Lp but not for absorption. $\sigma^2(I) = \sigma^2_{cs}(I) + (pI)^2$ with $p = 0\cdot04$. Accurate cell parameters were calculated from the setting angles of 25 reflections of crystal 2 with $9\cdot0 \leq \theta \leq 19\cdot2°$ using the *SET*4 method (Boer & Duisenberg, 1984). The two data sets were merged resulting in a set of 1275 unique reflections $[I > 2\cdot5\sigma(I)]$ used in the structure determination. All non-H atoms were found by direct methods (*SHELXS*86, Sheldrick, 1986) in space group $P1$. Space group $P\overline{1}$ was deduced from the structure. The structure was refined on F by full-matrix least-squares procedures using anisotropic thermal parameters for all non-H atoms (*SHELX*76, Sheldrick, 1976). The hydroxyl H atom was located from a difference Fourier map, and its positional and isotropic thermal parameters were refined. All other H atoms were introduced at calculated positions (C—H = 0·98 Å) and refined in the riding mode on their carrier atoms with a common isotropic thermal parameter. Subsequent cycles of difference Fourier maps revealed disorder of C4, C5, C8, C9 and C10, which is the result of partial substitution of one enantiomer by the other. The C atoms of the part with smaller population factor [0·231 (7)] were refined with isotropic temperature factors. Final convergence was reached at $R = 0\cdot049$ [$wR = 0\cdot052$, $w = 1/\sigma^2(F)$; $S = 0\cdot20$; $(\Delta/\sigma)_{max} = 0\cdot005$; number of refined parameters = 135]. No residual density outside the range $-0\cdot16$ and $0\cdot14$ e Å^{-3}. Scattering factors from Cromer & Mann (1968), anomalous-dispersion corrections from Cromer & Liberman (1970). The final atomic coordinates and equivalent isotropic temperature factors of the higher occupation form are listed in Table 1.* The program package *EUCLID* (Spek, 1982) was used for geometrical calculations and illustrations. All calculations were carried out on a MicroVAXII.

Related literature. A view of the molecule with the adopted numbering scheme is given in Fig. 1 and a projection of the structure down the *a* axis in Fig. 2. The bond distances and angles and angles involving non-H atoms of the higher occupation form are tabulated in Table 2; they are within normal ranges. The observed disorder is the result of substitution of one enantiomer on the position of another, made possible because of the geometrical similarity between the enantiomers, in which the isopropenyl group is equatorially attached to the cyclohexene ring. The same similarity is found for carvoxime, a methyl analogue of perillartine (Kroon, van Gurp,

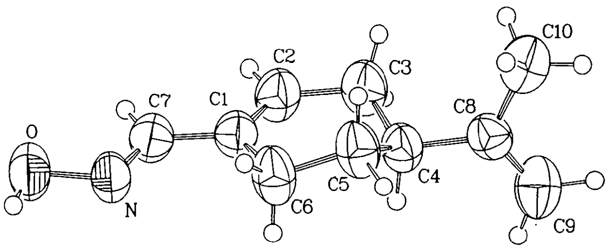

Fig. 1. *ORTEP* drawing of the molecule with higher occupation factor, with adopted labeling. H atoms are displayed as circles of arbitrary radius.

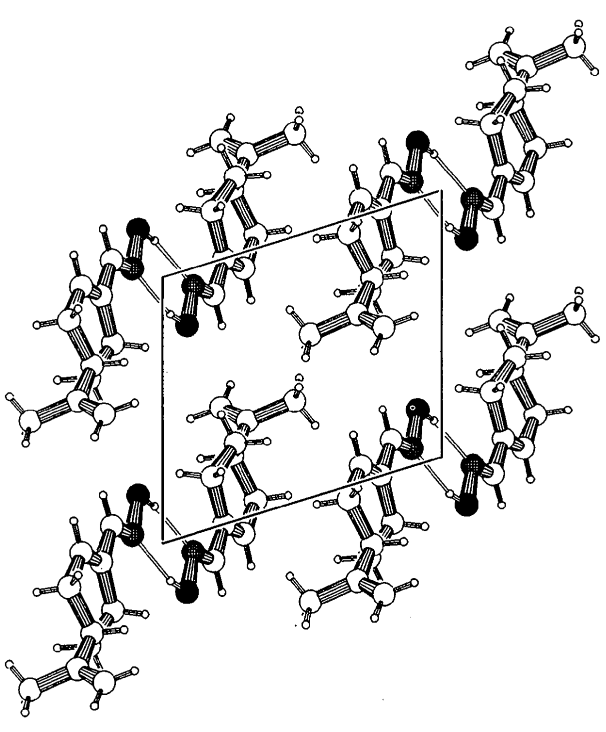

Fig. 2. Projection of the structure down the *a* axis showing the hydrogen-bonded dimers.

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* Lists of anisotropic thermal parameters, parameters for atoms with minor occupancy, H-atom positions, bond angles, distances and torsion angles and a list of structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52616 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances* (Å), *bond angles* (°), *torsion angles* (°) *and hydrogen-bond geometry*

O—N	1·410 (2)	C(4)—C(5)	1·496 (4)
N—C(7)	1·272 (3)	C(4)—C(8)	1·512 (5)
C(1)—C)2)	1·323 (3)	C(5)—C(6)	1·518 (4)
C(1)—C(6)	1·499 (3)	C(8)—C(9)	1·301 (8)
C(1)—C(7)	1·451 (3)	C(8)—C(10)	1·538 (9)
C(2)—C(3)	1·494 (3)	O—H(991)	0·84 (3)
C(3)—C(4)	1·521 (4)		

O—N—C(7)	111·8 (2)	C(5)—C(4)—C(8)	116·4 (3)
C(2)—C(1)—C(6)	121·5 (2)	C(4)—C(5)—C(6)	111·6 (2)
C(2)—C(1)—C(7)	120·1 (2)	C(1)—C(6)—C(5)	112·0 (2)
C(6)—C(1)—C(7)	118·5 (2)	N—C(7)—C(1)	120·7 (2)
C(1)—C(2)—C(3)	125·0 (2)	C(4)—C(8)—C(9)	120·9 (5)
C(2)—C(3)—C(4)	111·6 (2)	C(4)—C(8)—C(10)	120·9 (4)
C(3)—C(4)—C(5)	110·1 (2)	C(9)—C(8)—C(10)	118·2 (5)
C(3)—C(4)—C(8)	112·0 (3)	N—O—H(991)	98 (2)

O—N—C(7)—C(1)	178·4 (2)	C(2)—C(3)—C(4)—C(8)	−175·4 (3)
C(6)—C(1)—C(2)—C(3)	1·0 (3)	C(3)—C(4)—C(5)—C(6)	61·9 (4)
C(7)—C(1)—C(2)—C(3)	−179·0 (2)	C(8)—C(4)—C(5)—C(6)	−169·3 (3)
C(2)—C(1)—C(6)—C(5)	14·9 (3)	C(3)—C(4)—C(8)—C(9)	−107·7 (5)
C(7)—C(1)—C(6)—C(5)	−165·2 (2)	C(3)—C(4)—C(8)—C(10)	71·0 (5)
C(2)—C(1)—C(7)—N	177·5 (2)	C(5)—C(4)—C(8)—C(9)	124·4 (5)
C(6)—C(1)—C(7)—N	−2·4 (3)	C(5)—C(4)—C(8)—C(10)	−56·9 (6)
C(1)—C(2)—C(3)—C(4)	14·0 (3)	C(4)—C(5)—C(6)—C(1)	−46·2 (4)
C(2)—C(3)—C(4)—C(5)	−44·3 (3)	H(991)—O—N—C(7)	173 (2)

Oonk, Baert & Fouret, 1976). Indeed a comparable substitution disorder is found in the crystal structure of a mixed (+) and (±) carvoxime crystal (Baert, Fouret, Oonk & Kroon, 1978).

The molecules are connected in the structure by two symmetry-related O—H···N-type hydrogen bonds, O···N 2·830 (2) Å, O—H···N 159 (3)°. In both carvoxime structures mentioned above and in the structure of racemic carvoxime (Oonk & Kroon, 1976) the same six-membered cyclic hydrogen-bonded dimer is reported.

In order to identify the origin of the sweet taste in terms of the so-called *A*H—*B* model of Shallenberger & Acree (1967), a systematic search of possible hydrogen-bond donors and acceptors was performed. This revealed the C7H—O moiety with a C···O distance of 2·22 Å as the only candidate.

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Structure of 5′-*O*-Sulfamoylribavirin, an Antiparasitic Agent

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Abstract. 1-(5-*O*-Sulfamoyl-β-D-ribofuranosyl)-1*H*-1,2,4-triazole-3-carboxamide, $C_8H_{13}N_5O_7S$, M_r = 323·28, monoclinic, $P2_1$, a = 4·9405 (4), b = 9·1804 (11), c = 14·124 (2) Å, β = 93·973 (6)°, V = 639·06 (13) Å^3, Z = 2, D_x = 1·680 g cm^{-3}, Cu $K\alpha$ (λ = 1·54178 Å), μ = 26·573 cm^{-1}, $F(000)$ = 336, T = 295 K, R = 0·0224 for 2629 reflections ($F \geq 4\sigma_F$). The sugar conformation and puckering parameters are $^3T_2$ (C3′-*endo*/C2′-*exo*), P = 2·6° and τ_m = 40·2°. The C5′—O5′ side-chain orientation is *gauche*$^-$–*gauche*$^+$ [φ_{OO} = −60·9 (2); φ_{CO} = 57·4 (2)°]. The glycosylic torsion angle (N2—N1—C1′—O4′) is

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