O(22)···N(4), H(22)···N(4) and O(22)—H(22) distances in the α-epoxide are 2·737 (6), 1·83 (5) and 0·97 (7) Å respectively and the angle subtended at H(22) is 154 (4)°; the corresponding values in the β-epoxide are 2·849 (3), 2·01 (3) and 0·90 (4) Å and 155 (2)°. This interaction links the alkaloid molecules into chains in the α-epoxide crystal similar to the packing mode observed in the monocrotaline crystal. However, the additional hydrogen bonding in the β-epoxide monohydrate structure, in which each water links three alkaloid molecules, results in a three-dimensional network of hydrogen bonding. The water oxygen is the acceptor in the hydrogen bond with O(21); O(21)···O(*W*), H(21)···O(*W*), O(21)—H(21) distances are 2·773 (4), 1·94 (4) and 0·85 (5) Å respectively and the angle at H(21) is 166 (3)°. In the two other interactions the water oxygen is the donor atom; for the interaction with the carbonyl oxygen of the primary ester moiety the O(*W*)···O(20), H(1*W*)···O(20) and O(*W*)—H(1*W*) distances have the respective values 2·907 (4), 2·09 (4) and 0·87 (5) Å and the angle at H(1*W*) is 156 (3)°. For the interaction with the hydroxyl oxygen at C(13), the O(*W*)···O(22), H(2*W*)···O(20) and O(*W*)—H(2*W*) distances are 2·803 (3), 1·79 (5) and 1·04 (8) Å respectively and the angle at H(2*W*) is 164 (4)°.

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Structure of (−)-Epicatechin: (2*R*,3*R*)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-3,5,7-triol, $C_{15}H_{14}O_6$

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Abstract. $M_r = 290{\cdot}28$, orthorhombic, $P2_12_12_1$, $a = 6{\cdot}702$ (1), $b = 13{\cdot}273$ (1), $c = 14{\cdot}227$ (2) Å, $U = 1265{\cdot}6$ (3) Å^3, $Z = 4$, $D_x = 1{\cdot}523$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}74$ cm^{-1}, $F(000) = 608$, $T = 295$ K, $R = 0{\cdot}052$ for 623 reflexions [$I > 1{\cdot}5\sigma(I)$]. The heterocyclic ring is in a half-chair conformation. All oxygen atoms are involved in hydrogen bonds. Interaction between the OH groups of dihydroxyphenyl and 3,5,7-trihydroxybenzopyran residues, O(5)—H···O(4), connects molecules along **b** to form infinite chains. Parallel chains related by 2_1 axes along **b** are connected through O(3)—H···O(2) bonds between 3,5,7-trihydroxybenzopyran residues and O(2)—H···O(5) bonds in the *ab* plane. The O(2) hydroxyl group also exhibits an intramolecular contact to the heterocyclic O(1) forming a bifurcated hydrogen bond with O(5) as does O(5)—H with O(6) (both of the 3,4-dihydroxyphenyl residue). A weak interaction, O(6)—H···O(1), completes this bonding in a three-dimensional network.

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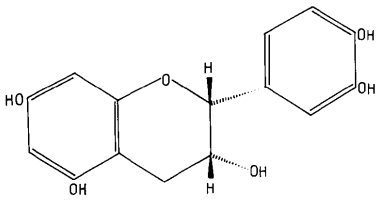
Introduction. Many plants within a wide variety of plant families accumulate epicatechin and catechin (Hegnauer, 1962–1973; Karrer, 1976). As a consequence, these compounds occur frequently in extracts from medicinal plants.



As such, these constituents may contribute to biological effects of such pharmaceutical preparations. Of the possible diastereoisomers of these compounds, phytochemical studies show that (−)-epicatechin and (+)-catechin appear to be the most abundantly occurring configurations in the living plant (Hegnauer, 1962–1973).

Many interesting biological activities of the catechins and related flavonoids in *in vitro* and *in vivo* experiments have been reported in the past fifty years (Böhm, 1967; Farkas, Gábor & Kállay, 1973, 1977). Some recent investigations have been focused on the relations between structure characteristics within a series of flavonoids and their specific activity on biological systems (Middleton, Drzewiecki, Lee, Busse, Schwartz, Sills, Malolepszy, Macander, Fanning, Ogra & Kaul, 1982). Specific structure–activity relationship could be demonstrated, for example, in effects on the arachidonic-acid metabolism, in the inhibitory effect on cyclic AMP phosphodiesterase and in effects on various cell-membrane–ligand systems (Middleton *et al.*, 1982; Beretz, Anton & Stoclet, 1978; Wurm, Baumann & Geres, 1982). Recently, we found structure-related effects on both the classical and the alternative pathways of human complement (Labadie, van Putten, Kroes & van Meer, 1984).

The marked differences in the inhibitory activity between the diastereoisomers of epicatechin and catechin were striking and prompted us to further structure analysis. The conformation and absolute configuration of 8-bromo-*O*-methyl-(+)-catechin have been described by Engel, Hattingh, Hundt & Roux (1978). The present paper reports the results of an X-ray analysis of (−)-epicatechin.

Experimental. Small colourless transparent crystal selected from a commercial sample (Roth). Enraf–Nonius CAD-4F diffractometer, ω-scan mode ($\theta_{max} = 22°$), Zr-filtered Mo $K\alpha$ radiation aiming at a constant $\sigma(I)/I$ ratio of 0·01; crystal dimensions 0·12 × 0·12 × 0·25 mm; 938 independent reflexions ($0 < h < 7$, $0 < k < 13$, $0 < l < 14$) of which 623 [$I > 1{\cdot}5\sigma(I)$] used in calculations; two reference reflexions ($\bar{1}04$: $\sigma = 0{\cdot}50\%$; $10\bar{2}$: $\sigma = 0{\cdot}66\%$) showed small decay of 1% during 14 h of X-ray exposure time; cell constants derived by least squares from diffractometer settings of 14 reflexions in the range $3 < \theta < 9°$. Lorentz and polarization corrections. Structure solved by *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) (based on 221 reflexions having $|E| \geq 1{\cdot}20$). Difference Fourier synthesis located H atoms of OH groups, others introduced at calculated positions and refined in riding mode on carrier atoms. Peak at 1·30 Å from O(6) in the direction of O(1) observed, but since its refinement did not improve the geometry of the O(6) hydroxyl group, H(6) was not included in the final refinement cycles. Full-matrix least-squares technique minimizing $\sum w(\Delta F)^2$ with $w = 1$. Scale factor, atomic coordinates of all atoms excluding H(2)–H(5), anisotropic thermal parameters for non-hydrogen atoms, and two isotropic thermal parameters for H atoms bonded to C (U = 0·041 Å^2) and O (U = 0·057 Å^2) refined (192 variables). H-atom positions H(2)–H(5) are of low accuracy in view of the ratio of observations to the number of variables (~3). 002 excluded in final stages of refinement [$\Delta F/\sigma(F) = 8{\cdot}30$]. Large ΔF might be explained by extinction effect. Max. Δ/σ on coordinates in final refinement cycle 0·04 [for O(1)]; anisotropic thermal parameters in usual range; final $R = 0{\cdot}0516$, $wR = 0{\cdot}0512$, $S = 1{\cdot}22$; max. and min. residual densities 0·10 and −0·10 e Å^{-3}; scattering factors from Cromer & Mann (1968) and (for H) Stewart, Davidson & Simpson (1965). In-house DG-Eclipse S/230 minicomputer using programs of *ILIAS* package [an adaptation and extension by ALS of *SHELX*76 (Sheldrick, 1976)], or the CDC-Cyber 175 of the University of Utrecht with programs of the *EUCLID* package [calculation of geometrical data and preparation of illustrations including an extended version of the program *PLUTO* (Spek, 1982)] were used.*

Discussion. Final atomic parameters are given in Table 1.* Bond lengths and angles and selected torsion angles describing the conformation of the molecule are listed in Table 2. A *PLUTO* drawing of a molecule with the atomic numbering scheme is shown in Fig. 1. Hydrogen bonds are listed in Table 3. The molecular packing is illustrated in Fig. 2.

The interatomic distances and angles do not reveal any exception to the standard values. The C—O bond in the flavan ring is asymmetrical [C(2)—O(1), 1·46 (1); C(9)—O(1), 1·39 (1) Å] owing to the effect of conjugation on the C(9) side (Table 2). The natural substance described as (−)-epicatechin (Haslam, 1982)

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond lengths and angles involving H have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39651 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final atomic coordinates and equivalent isotropic thermal parameters*

	x	y	z	U_{eq}(Å²)*
O(1)	0·154 (1)	0·0184 (4)	0·9023 (5)	0·035 (2)
O(2)	0·364 (1)	0·0774 (4)	0·7306 (4)	0·033 (2)
O(3)	0·646 (1)	−0·2310 (5)	0·8316 (5)	0·039 (2)
O(4)	−0·011 (1)	−0·3268 (4)	0·9213 (5)	0·035 (2)
O(5)	−0·040 (1)	0·4789 (4)	0·8487 (6)	0·053 (2)
O(6)	0·314 (1)	0·4609 (4)	0·9497 (5)	0·050 (2)
C(2)	0·313 (1)	0·0938 (6)	0·9011 (7)	0·029 (2)
C(3)	0·459 (1)	0·0729 (7)	0·8209 (7)	0·033 (2)
C(4)	0·561 (1)	−0·0269 (6)	0·8374 (7)	0·030 (2)
C(5)	0·453 (2)	−0·2085 (7)	0·8565 (7)	0·029 (2)
C(6)	0·316 (1)	−0·2821 (7)	0·8774 (6)	0·025 (2)
C(7)	0·129 (1)	−0·2542 (7)	0·9038 (7)	0·029 (2)
C(8)	0·075 (1)	−0·1540 (6)	0·9151 (7)	0·025 (2)
C(9)	0·220 (2)	−0·0807 (7)	0·8941 (7)	0·031 (2)
C(10)	0·409 (2)	−0·1054 (6)	0·8632 (7)	0·033 (2)
C(11)	0·207 (1)	0·1954 (6)	0·8901 (6)	0·024 (2)
C(12)	0·305 (1)	0·2798 (6)	0·9278 (6)	0·027 (2)
C(13)	0·225 (1)	0·3748 (6)	0·9137 (7)	0·026 (2)
C(14)	0·046 (2)	0·3855 (6)	0·8639 (7)	0·033 (2)
C(15)	−0·048 (2)	0·3021 (7)	0·8309 (7)	0·036 (2)
C(16)	0·029 (1)	0·2073 (6)	0·8407 (7)	0·029 (2)

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

Table 2. *Selected intramolecular geometry*

Bond distances (Å)

O(1)–C(2)	1·46 (1)	C(5)–C(6)	1·38 (1)
O(1)–C(9)	1·39 (1)	C(5)–C(10)	1·40 (1)
O(2)–C(3)	1·44 (1)	C(6)–C(7)	1·36 (1)
O(3)–C(5)	1·38 (1)	C(7)–C(8)	1·39 (1)
O(4)–C(7)	1·37 (1)	C(8)–C(9)	1·41 (1)
O(5)–C(14)	1·38 (1)	C(9)–C(10)	1·38 (1)
O(6)–C(13)	1·39 (1)	C(11)–C(16)	1·39 (1)
C(2)–C(11)	1·53 (1)	C(11)–C(12)	1·41 (1)
C(2)–C(3)	1·53 (1)	C(12)–C(13)	1·38 (1)
C(3)–C(4)	1·51 (1)	C(13)–C(14)	1·40 (1)
C(4)–C(10)	1·50 (1)	C(14)–C(15)	1·36 (1)
		C(15)–C(16)	1·37 (1)

Bond angles (°)

C(2)–O(1)–C(9)	114·6 (7)	C(8)–C(9)–C(10)	122·5 (8)
C(3)–C(2)–C(11)	112·4 (8)	O(1)–C(9)–C(10)	122·7 (8)
O(1)–C(2)–C(3)	110·5 (7)	C(5)–C(10)–C(9)	116·5 (9)
O(1)–C(2)–C(11)	105·3 (7)	C(4)–C(10)–C(5)	121·1 (9)
O(2)–C(3)–C(2)	112·2 (8)	C(4)–C(10)–C(9)	122·4 (8)
O(2)–C(3)–C(4)	112·2 (8)	C(12)–C(11)–C(16)	120·2 (8)
C(2)–C(3)–C(4)	109·5 (8)	C(2)–C(11)–C(16)	123·3 (8)
C(3)–C(4)–C(10)	109·7 (8)	C(2)–C(11)–C(12)	116·4 (8)
C(6)–C(5)–C(10)	122·5 (9)	C(11)–C(12)–C(13)	119·4 (9)
O(3)–C(5)–C(6)	122·1 (8)	O(6)–C(13)–C(12)	122·2 (8)
O(3)–C(5)–C(10)	115·3 (9)	C(12)–C(13)–C(14)	119·8 (8)
C(5)–C(6)–C(7)	118·8 (9)	O(6)–C(13)–C(14)	118·0 (8)
C(6)–C(7)–C(8)	122·3 (9)	O(5)–C(14)–C(15)	119·0 (9)
O(4)–C(7)–C(8)	118·3 (8)	C(13)–C(14)–C(15)	119·3 (8)
O(4)–C(7)–C(6)	119·4 (8)	O(5)–C(14)–C(13)	121·7 (8)
C(7)–C(8)–C(9)	117·3 (9)	C(14)–C(15)–C(16)	123 (1)
O(1)–C(9)–C(8)	114·7 (8)	C(11)–C(16)–C(15)	118·7 (8)

Torsion angles (°)

O(1)–C(2)–C(3)–C(4)	−64 (1)
C(2)–C(3)–C(4)–C(10)	47 (1)
C(3)–C(4)–C(10)–C(9)	−18 (1)
C(4)–C(10)–C(9)–O(1)	1 (2)
O(1)–C(2)–C(11)–C(12)	152·2 (8)
O(1)–C(2)–C(3)–O(2)	61·3 (9)
C(3)–C(2)–C(11)–C(12)	−87 (1)
O(2)–C(3)–C(4)–C(10)	−78 (1)

was used in this study and according to this the (2*R*, 3*R*) enantiomer was selected (Fig. 1). The conformation of the heterocycle is a half-chair; O(1) and C(4) are coplanar with the C(5)–C(10) benzene ring within the limits of experimental error, whereas C(2) is 0·31 (2) above and C(3) 0·46 (2) Å below this plane. The values of the torsion angles about O(1)–C(2) and C(3)–C(4) give evidence for such a conformation (Table 2). The values of the Cremer & Pople (1975) ring-puckering analysis [atom sequence O(1), C(2), C(3), C(4), C(10), C(9); $Q = 0{\cdot}50\ (1)$ Å, $\theta = 131\ (1)$, $\varphi = 274\ (1)°$] correspond also to a half-chair conformation. The substituents at C(2) and C(3) are *cis* positioned.

The crystal packing is dominated by hydrogen bonds (Table 3). The O(2) and O(5) hydroxyl groups exhibit both donor and acceptor functions whereas O(4) acts solely as an acceptor. The hydrogen bond O(5)–H···O(4), connects the molecules into an infinite chain along the **b** direction. Chains related by 2_1 axes parallel to **b** are joined through O(2)–H···O(3), forming a two-dimensional pattern in the *ab* plane. The O(5)–H group with its acceptor function in the contact O(2)–H···O(5), together with two already mentioned hydrogen bonds, builds a spiral along **a**. The O(2)–H group is also involved as donor in an intramolecular contact to the heterocycle oxygen O(1), sharing H(2) with O(5)

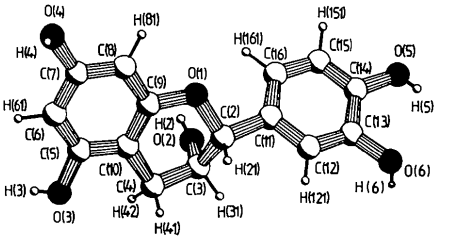


Fig. 1. A *PLUTO* drawing of the molecule with the atom numbering. The H atom bonded to O(6) was not determined.

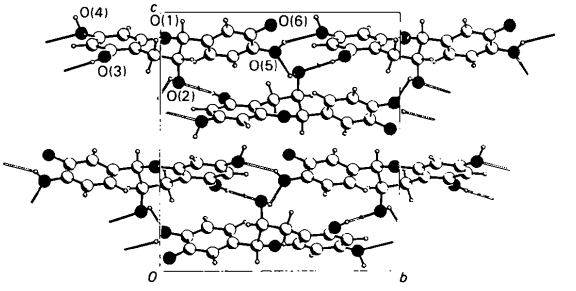


Fig. 2. A view of the structure down **a** illustrating the hydrogen bonds. The intramolecular hydrogen bonds O(2)–H···O(1) and O(5)–H···O(6) and the weak interaction O(6)···O(1) are marked by dotted lines. The hydrogen bond O(3)–H···O(2), which connects molecules translated in the **a** direction is marked with ~.

Table 3. *Hydrogen bonds*

D—H···*A*	*D*···*A* (Å)	*D*—H (Å)	H···*A* (Å)	∠*D*—H···*A* (°)	Symmetry operation on *A*
O(2)—H(2)···O(1)	2·92 (1)	0·76	2·42	124	x, y, z
O(2)—H(2)···O(5)	2·78 (1)	0·76	2·23	128	$-x, y-\frac{1}{2}, \frac{3}{2}-z$
O(3)—H(3)···O(2)	2·69 (1)	0·74	1·97	169	$1-x, y-\frac{1}{2}, \frac{3}{2}-z$
O(5)—H(5)···O(4)	2·78 (1)	0·77	2·15	140	$x, y+1, z$
O(5)—H(5)···O(6)	2·78 (1)	0·77	2·38	113	x, y, z
O(6)—H···O(1)	3·12 (1)				$\frac{1}{2}+x, \frac{1}{2}-y, 2-z$

in a bifurcated hydrogen bond. The geometrical parameters of this bond (Table 3) were analysed according to the criteria given by Newton, Jeffrey & Takagi (1979). The function of the O(6)—H group is somewhat uncertain because no reliable hydrogen position could be secured. It is quite common that aromatic derivatives with substituents with donor–acceptor properties in the *ortho* position exhibit intramolecular hydrogen bonds (Pimentel & McClellan, 1960; Schuster, Zundel & Sandorfy, 1976). In such a case a bifurcated hydrogen bond can be proposed in which H(5) would be shared between O(4) and O(6) (Table 3). The two-dimensional layers of hydrogen-bonded molecules are linked in the **c** direction *via* the weak interaction O(6)—H···O(1) (Fig. 2).

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Acta Cryst. (1984). C**40**, 2071–2074

The Structure of 5,5-Diphenyl-1,3-oxazolidine-2,4-dione, $C_{15}H_{11}NO_3$

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Abstract. $M_r = 253{\cdot}26$, monoclinic, $P2_1/c$, $a = 12{\cdot}473\ (8)$, $b = 6{\cdot}025\ (1)$, $c = 16{\cdot}371\ (11)$ Å, $\beta = 90{\cdot}57\ (3)°$, $V = 1230\ (1)$ Å^3, $Z = 4$, $F(000) = 528$, $D_x = 1{\cdot}37$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71069$ Å, $\mu = 1{\cdot}04$ cm^{-1}, $T = 173\ (5)$ K, $R = 0{\cdot}092$, $R_w = 0{\cdot}042$, 1779 observed reflections. The angle between the two phenyl rings is $79{\cdot}7\ (5)°$ and the angles between the oxazolidinedione ring and each of the two phenyl rings

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