the N(1)C(2)S(3)S(8) moiety – gains some π-bond character [1·725 (1) Å and it is accompanied by a strong N(1)—C(2) multiple bond 1·321 (2) Å]. The nearly coplanar N(1)C(2)S(3)S(8) moiety imposes an envelope (1,2-diplanar) conformation on the 1,3-thiazine ring with C(4a) at the flap. A mirror plane (C_s) indicated by the low asymmetry factor (Kálmán, Czugler & Simon, 1982) $fC_s = 0{\cdot}017$ (4) Å [computed from the puckering parameters of Cremer & Pople (1975): $Q = 0{\cdot}488$ (2) Å, $\varphi = 236{\cdot}8$ (4) and $\theta = 50{\cdot}3$ (3)°] bisects C(2) and C(4a). In contrast with the analogous tetrahydro-1,3-oxazin-2-one and -thione derivatives fused with cyclopentane rings (Argay, Kálmán, Kapor, Stájer & Bernáth 1985; Stanković, Kapor, Ribár, Kálmán, Argay, Karanović, Stájer & Bernáth, 1985), in compound (2*a*) the *cis*-fused cyclopentane ring (Fig. 1), albeit assuming an almost perfect half-chair conformation [$Q = 0{\cdot}403$ (3) Å, $\varphi = 162{\cdot}6$ (5)°] with twofold symmetry (C_2) bisecting C(6) [$fC_2 = 0{\cdot}003$ (4) Å for C(6)], does not shift the conformation of the hetero ring towards a C(4a)—C(7a) half chair. The least-squares plane of the phenyl ring bound *pseudoequatorially* to the hetero ring makes a dihedral angle of −62·45 (8)° with that of the N(1)-C(2)S(3)S(8) moiety. The hydroxyl group orientated *pseudoaxially* to the hetero ring forms an intermolecular hydrogen bond with S(8) at $x, -y, z-\frac{1}{2}$ with the following parameters: O···S = 3·303 (2), H···S = 2·21 (1) Å, ∠OH···S = 154 (2)°.

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Structure of 1,2-Dihydro-1,2,2-tris[(2-hydroxyphenyl)methyl]-3*H*-indol-3-one (Uvarindole D)*

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Abstract. $C_{29}H_{25}NO_4$, $M_r = 451{\cdot}53$, monoclinic, $P2_1/n$, $a = 14{\cdot}031$ (3), $b = 10{\cdot}031$ (4), $c = 16{\cdot}491$ (5) Å, $\beta = 96{\cdot}51$ (3)°, $U = 2306{\cdot}1$ Å^3, $Z = 4$, $D_x = 1{\cdot}301$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}49$ cm^{-1}, $F(000) = 952$, $T = 293$ (2) K, final $R = 0{\cdot}044$ for 2673 unique reflections considered observed with $F_o > 3\sigma(F_o)$. Three *o*-hydroxybenzyl groups with nearly planar rings are 1,2,2-attached to the indole nucleus, which has longer than normal C(2)—C(3) and C(3)—O(3) bonds and twists of up to 15° about heterocyclic ring bonds. Exit bonds from the heterocycle take up conformations that reduce crowding. Two OH groups hydrogen-bond to the carbonyl oxygen atom, while one of these phenolic oxygen atoms also accepts a hydrogen bond from the third OH.

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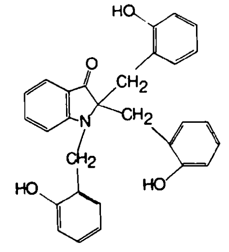
Introduction. Extraction of stem bark of *Uvaria angolensis* collected in Tanzania has yielded four novel benzylated indoles (Waterman & Mohammad, 1984). One of these, uvarindole D, was shown by spectroscopic analysis to contain three *o*-hydroxybenzyl substitutents and a carbonyl group. Correlation of spectral data with that obtained for the other uvarindoles and from indol-2-one and indol-3-one alkaloids led to the tentative assignment of structure (1) for uvarindole D. In order to prove conclusively the location of these groups on the indole nucleus and also to ascertain how the aromatic rings are arranged for good intramolecular and intermolecular packing, a crystal structure determination was undertaken.



(1)

Experimental. Yellow crystals of uvarindole D were grown from chloroform; a specimen 0·75 × 0·25 × 0·25 mm was selected. Unit-cell dimensions from least-squares analysis of setting angles of 25 reflections, $9{\cdot}90 \leq \theta \leq 14{\cdot}31°$, graphite-monochromated Mo $K\alpha$ radiation, Enraf–Nonius CAD-4 diffractometer. Intensity data obtained by ω–2θ scans with ω scan range = $(0{\cdot}96 + 0{\cdot}35\tan\theta)°$ and ω scan speed 0·6 to 2·8° min^{-1} depending on intensity. Three orientation and intensity standard reflections re-measured every 100 reflections and 2 h respectively; no significant crystal decay and slight movement satisfactorily corrected by one redetermination of the orientation matrix. 4481 reflections with $-16 \leq h \leq 0$, $0 \leq k \leq 11$, $-19 \leq l \leq 19$ measured in the range $2 \leq \theta \leq 25°$, assigned estimated standard deviations σ based on counting statistics and an allowance of $0{\cdot}02F_o$ for the minimum expected experimental instability, and merged; 4039 unique reflections ($R_{\rm int} = 0{\cdot}028$), 2673 observed [$F_o > 3\sigma(F_o)$]. Data corrected for Lorentz–polarization effects assuming an ideally imperfect monochromator, but not for absorption in view of the low absorbing power of the crystal (range of transmission factors along straight paths 0·964–0·988).

Phase determination by the EEES procedure in *SHELX* (Sheldrick, 1976), all non-hydrogen atoms found in an *E* map, all hydrogen atoms subsequently located in a difference electron density map. Final refinement with *SHELX* and its stored scattering factors (Stewart, Davidson & Simpson, 1965; Cromer & Mann, 1968) adjusted coordinates and anisotropic thermal parameters for non-hydrogen atoms; in alternate cycles coordinates and isotropic temperature factors of hydrogen atoms were refined instead. In the last two cycles no parameter of either sort shifted by more than 0·19 e.s.d. The function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w = k/[\sigma^2(F_o) + gF_o^2]$ and g converged to 0·003073. Final discrepancy indices were $R = 0{\cdot}044$, $wR = 0{\cdot}062$; and no peak on a difference Fourier synthesis exceeded 0·16 e Å^{-3}.

Discussion. The structure of uvarindole D is shown in Fig. 1 together with its numbering scheme. Coordinates and (equivalent) isotropic temperature factors of all atoms are listed in Table 1.* Bond lengths, bond angles, and selected torsion angles are displayed in Table 2.

The N(1)—C(9) and C(3)—C(4) bond distances of 1·371 (3) and 1·435 (3) Å respectively are shorter than would be expected for single bonds (*International Tables for X-ray Crystallography,* 1968). Furthermore, in the benzene ring of the indole nucleus the C(4)—C(5), C(6)—C(7), C(8)—C(9) and C(4)—C(9) distances are significantly longer than the C(5)—C(6) and C(7)—C(8) bond lengths, the former distances being 1·392 (4), 1·403 (4), 1·401 (3) and 1·406 (3) Å respectively, and the latter distances being 1·371 (4) and 1·370 (4) Å. This could be due to conjugation through most of the 'indole' ring signified by resonance structure (2*b*) as

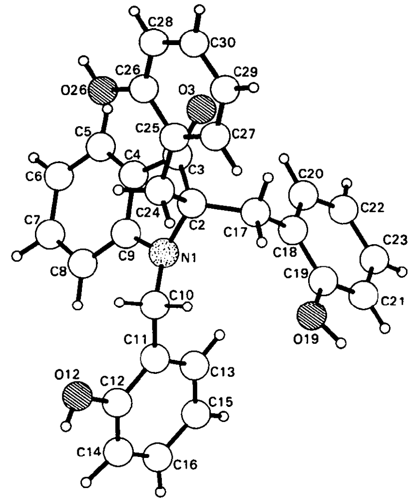


Fig. 1. *PLUTO* (Motherwell & Clegg, 1978) drawing of the molecule projected onto its least-squares plane, showing the crystallographic numbering scheme.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43374 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

well as (2*a*). However, if contributing structure (2*b*) were dominant then one might expect the C(3)—O(3) bond length to be even longer than the observed 1·236 (2) Å, although it is already considerably longer than the carbonyl bond distances reported for acetophenone (Tanimoto, Kobayashi, Nagakura & Saito, 1973), *p*-aminoacetophenone (Haisa, Kashino, Yuasa & Akigawa, 1976), and isatin (Goldschmidt & Llewellyn, 1950). Another predisposing factor to the shorter C(3)—C(4) bond length may be the steric crowding at C(2), causing C(2)—C(3) to stretch to 1·522 (3) Å to accommodate the large C(2) substituents. The decreased bond order here could be compensated by a shorter, stronger C(3)—C(4) bond.

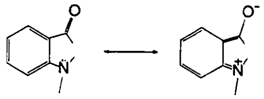
(2*a*) (2*b*)

Table 1. *Atom positional parameters for uvarindole D (fractional coordinates* $\times 10^4$ *for non-hydrogen atoms;* $\times 10^3$ *for hydrogen atoms) and equivalent isotropic* ($\times 10^4$) *or isotropic* ($\times 10^3$) *temperature factors, with e.s.d.'s in parentheses*

$$U_{\rm eq} = \tfrac{1}{3}(U_{11} + U_{22} + U_{33} + 2U_{13}\cos\beta).$$

	x	y	z	$U_{\rm iso}$(Å^2)
N(1)	4437 (1)	−43 (2)	6810 (1)	312 (5)
C(2)	3805 (2)	1047 (2)	6471 (2)	289 (6)
C(3)	4496 (2)	2216 (2)	6471 (1)	309 (7)
C(4)	5453 (2)	1692 (2)	6610 (1)	352 (7)
C(5)	6340 (2)	2296 (3)	6570 (2)	493 (9)
C(6)	7151 (2)	1527 (3)	6691 (2)	572 (10)
C(7)	7070 (2)	160 (3)	6850 (2)	519 (9)
C(8)	6206 (2)	−452 (3)	6901 (2)	420 (8)
C(9)	5373 (2)	327 (2)	6784 (1)	326 (7)
C(10)	4110 (2)	−1422 (2)	6721 (1)	366 (7)
C(11)	4532 (2)	−2317 (2)	7402 (1)	341 (7)
C(12)	4808 (2)	−3611 (2)	7248 (1)	338 (7)
C(13)	4626 (2)	−1886 (3)	8206 (2)	462 (8)
C(14)	5178 (2)	−4440 (3)	7880 (2)	448 (8)
C(15)	4986 (2)	−2703 (3)	8834 (2)	547 (10)
C(16)	5264 (2)	−3982 (3)	8668 (2)	539 (10)
C(17)	3463 (2)	707 (2)	5555 (1)	350 (7)
C(18)	2935 (2)	1763 (2)	5038 (1)	352 (7)
C(19)	3434 (2)	2647 (3)	4586 (1)	390 (8)
C(20)	1943 (2)	1832 (3)	4940 (2)	486 (9)
C(21)	2940 (2)	3548 (3)	4051 (2)	513 (9)
C(22)	1456 (2)	2727 (4)	4410 (2)	629 (11)
C(23)	1958 (2)	3575 (3)	3967 (2)	625 (11)
C(24)	2950 (2)	1286 (2)	6947 (1)	323 (7)
C(25)	3136 (2)	1516 (2)	7858 (1)	320 (7)
C(26)	2736 (2)	663 (2)	8386 (2)	384 (7)
C(27)	3616 (2)	2626 (3)	8208 (2)	412 (8)
C(28)	2772 (2)	916 (3)	9206 (2)	566 (10)
C(29)	3664 (2)	2887 (3)	9032 (2)	517 (9)
C(30)	3224 (2)	2043 (4)	9531 (2)	608 (11)
O(3)	4229 (1)	3383 (1)	6365 (1)	384 (5)
O(12)	4729 (1)	−4042 (2)	6454 (1)	434 (5)
O(19)	4407 (1)	2552 (2)	4672 (1)	489 (6)
O(26)	2296 (1)	−450 (2)	8051 (1)	589 (7)
H(5)	632 (2)	319 (3)	642 (2)	50 (7)
H(6)	786 (3)	194 (4)	671 (2)	101 (12)
H(7)	766 (2)	−43 (3)	689 (2)	56 (7)
H(8)	618 (2)	−141 (3)	705 (2)	63 (8)
H(10*A*)	427 (2)	−175 (2)	622 (1)	38 (6)
H(10*B*)	340 (2)	−137 (2)	673 (2)	49 (7)
H(12)	467 (2)	−486 (4)	640 (2)	95 (11)
H(13)	444 (2)	−101 (3)	830 (2)	56 (7)
H(14)	543 (2)	−537 (3)	772 (2)	60 (8)
H(15)	508 (2)	−234 (3)	940 (2)	78 (10)
H(16)	551 (2)	−454 (3)	913 (2)	66 (8)
H(17*A*)	302 (2)	−6 (2)	558 (2)	37 (6)
H(17*B*)	404 (2)	45 (2)	530 (1)	41 (6)
H(19)	467 (2)	307 (3)	435 (2)	60 (8)
H(20)	160 (2)	122 (3)	526 (2)	47 (7)
H(21)	325 (2)	415 (3)	374 (2)	67 (8)
H(22)	78 (2)	281 (3)	435 (2)	88 (10)
H(23)	165 (2)	426 (3)	358 (2)	79 (10)
H(24*A*)	248 (2)	51 (2)	687 (1)	44 (6)
H(24*B*)	263 (2)	202 (2)	669 (1)	39 (6)
H(26)	184 (3)	−85 (4)	837 (2)	110 (12)
H(27)	386 (2)	327 (2)	783 (1)	41 (6)
H(28)	247 (2)	36 (3)	955 (2)	73 (9)
H(29)	407 (2)	369 (3)	926 (2)	75 (9)
H(30)	327 (2)	218 (3)	1013 (2)	74 (9)

Table 2. *Bond distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses and selected torsion angles* (*e.s.d.* 0·4°) *for non-hydrogen atoms of uvarindole D*

N(1)—C(2)	1·478 (3)	C(13)—C(15)	1·371 (4)
C(2)—C(3)	1·522 (3)	C(14)—C(16)	1·370 (4)
C(2)—C(17)	1·568 (3)	C(15)—C(16)	1·377 (4)
C(2)—C(24)	1·525 (3)	C(17)—C(18)	1·501 (3)
C(3)—C(4)	1·435 (3)	C(18)—C(19)	1·396 (3)
C(3)—O(3)	1·236 (3)	C(18)—C(20)	1·385 (4)
C(4)—C(5)	1·392 (4)	C(19)—C(21)	1·392 (4)
C(4)—C(9)	1·406 (3)	C(19)—O(19)	1·360 (3)
C(5)—C(6)	1·371 (4)	C(20)—C(22)	1·379 (4)
C(6)—C(7)	1·403 (4)	C(21)—C(23)	1·369 (4)
C(7)—C(8)	1·370 (4)	C(22)—C(23)	1·368 (5)
C(8)—C(9)	1·401 (3)	C(24)—C(25)	1·513 (3)
C(9)—N(1)	1·371 (3)	C(25)—C(26)	1·384 (3)
N(1)—C(10)	1·460 (3)	C(25)—C(27)	1·393 (3)
C(10)—C(11)	1·505 (3)	C(26)—C(28)	1·371 (4)
C(11)—C(12)	1·387 (3)	C(26)—O(26)	1·362 (3)
C(11)—C(13)	1·387 (4)	C(27)—C(29)	1·378 (4)
C(12)—C(14)	1·387 (3)	C(28)—C(30)	1·374 (5)
C(12)—O(12)	1·372 (3)	C(29)—C(30)	1·374 (4)

C(2)—N(1)—C(9)	108·9 (2)	C(11)—C(12)—O(12)	118·4 (2)
C(2)—N(1)—C(10)	119·7 (2)	C(14)—C(12)—O(12)	120·8 (2)
C(9)—N(1)—C(10)	123·0 (2)	C(11)—C(13)—C(15)	121·5 (3)
N(1)—C(2)—C(3)	102·4 (2)	C(12)—C(14)—C(16)	119·8 (2)
N(1)—C(2)—C(17)	108·0 (2)	C(13)—C(15)—C(16)	119·7 (3)
N(1)—C(2)—C(24)	113·2 (2)	C(14)—C(16)—C(15)	120·2 (3)
C(3)—C(2)—C(17)	107·1 (2)	C(2)—C(17)—C(18)	118·1 (2)
C(3)—C(2)—C(24)	114·7 (2)	C(17)—C(18)—C(19)	120·4 (2)
C(17)—C(2)—C(24)	110·9 (2)	C(17)—C(18)—C(20)	121·8 (2)
C(2)—C(3)—C(4)	107·6 (2)	C(19)—C(18)—C(20)	117·6 (2)
C(2)—C(3)—O(3)	123·2 (2)	C(18)—C(19)—C(21)	120·4 (2)
C(4)—C(3)—O(3)	129·2 (2)	C(18)—C(19)—O(19)	117·3 (2)
C(3)—C(4)—C(5)	131·2 (2)	C(21)—C(19)—O(19)	122·2 (2)
C(3)—C(4)—C(9)	107·1 (2)	C(18)—C(20)—C(22)	121·8 (3)
C(5)—C(4)—C(9)	121·7 (2)	C(19)—C(21)—C(23)	120·1 (3)
C(4)—C(5)—C(6)	118·7 (3)	C(20)—C(22)—C(23)	119·7 (3)
C(5)—C(6)—C(7)	119·5 (3)	C(21)—C(23)—C(22)	120·4 (3)
C(6)—C(7)—C(8)	122·7 (2)	C(2)—C(24)—C(25)	118·6 (2)
C(7)—C(8)—C(9)	118·2 (2)	C(24)—C(25)—C(26)	119·6 (2)
C(4)—C(9)—C(8)	119·1 (2)	C(24)—C(25)—C(27)	123·7 (2)
C(4)—C(9)—N(1)	111·7 (2)	C(25)—C(26)—C(28)	122·3 (2)
C(8)—C(9)—N(1)	129·2 (2)	C(25)—C(26)—O(26)	116·7 (2)
N(1)—C(10)—C(11)	113·4 (2)	C(28)—C(26)—O(26)	121·1 (2)
C(10)—C(11)—C(12)	121·1 (2)	C(25)—C(27)—C(29)	121·8 (2)
C(10)—C(11)—C(13)	121·0 (2)	C(26)—C(28)—C(30)	120·0 (3)
C(12)—C(11)—C(13)	117·9 (2)	C(27)—C(29)—C(30)	119·9 (3)
C(11)—C(12)—C(14)	120·8 (2)	C(28)—C(30)—C(29)	119·5 (3)

C(17)—C(2)—C(3)—C(4)	−100·3	C(7)—C(8)—C(9)—N(1)	−179·4
C(24)—C(2)—C(3)—C(4)	136·2	C(8)—C(9)—N(1)—C(2)	−167·5
N(1)—C(2)—C(3)—C(4)	13·2	C(4)—C(9)—N(1)—C(2)	12·3
N(1)—C(2)—C(3)—O(3)	−167·0	C(2)—N(1)—C(10)—C(11)	−150·7
C(3)—C(2)—N(1)—C(9)	−15·3	N(1)—C(10)—C(11)—C(12)	102·8
C(3)—C(2)—N(1)—C(10)	−164·3	N(1)—C(2)—C(17)—C(18)	−170·7
C(2)—C(3)—C(4)—C(5)	171·1	C(2)—C(17)—C(18)—C(19)	91·5
C(2)—C(3)—C(4)—C(9)	−6·7	N(1)—C(2)—C(24)—C(25)	53·5
O(3)—C(3)—C(4)—C(5)	−8·7	C(2)—C(24)—C(25)—C(26)	−120·6
O(3)—C(3)—C(4)—C(9)	173·5	C(11)—C(12)—O(12)—H(12)	−154·6
C(3)—C(4)—C(5)—C(6)	−176·4	C(18)—C(19)—O(19)—H(19)	175·2
C(9)—C(4)—C(5)—C(6)	1·1	C(25)—C(26)—O(26)—H(26)	−159·2
C(3)—C(4)—C(9)—C(8)	176·5	C(11)—C(12)—C(14)—C(16)	0·6
C(3)—C(4)—C(9)—N(1)	−3·3	C(11)—C(13)—C(15)—C(16)	0·2
C(4)—C(5)—C(6)—C(7)	0·1	C(18)—C(19)—C(21)—C(23)	0·3
C(5)—C(6)—C(7)—C(8)	−0·8	C(18)—C(20)—C(22)—C(23)	0·0
C(6)—C(7)—C(8)—C(9)	0·4	C(25)—C(26)—C(28)—C(30)	−0·6
C(7)—C(8)—C(9)—C(4)	0·8	C(25)—C(27)—C(29)—C(30)	−0·5

There is approximately tetrahedral geometry at C(2) although the C(3)—C(2)—N(1) angle at 102·4 (2)° is below the tetrahedral value, probably to allow bond angles involving C(24) to exceed this value and make more room for the large C_7H_7O substituents. The C(24)—C(2)—C(3) angle is 114·7 (2)° and the C(24)—C(2)—N(1) angle is 113·2 (2)°. At N(1), the C(9)—N(1)—C(2) angle is 108·9 (2)°, which is similar to that reported in indole (Hanson, 1964) and indole-3-acetic acid (Karle, Britts & Gum, 1964). Although the C(9)—N(1)—C(10) and C(2)—N(1)—C(10) angles are larger at 123·0 (2) and 119·7 (2)° respectively, the sum of the bond angles at N(1) is 351·6 (3)°, indicating some degree of pyramidalization at N(1).

Torsion angles show that the benzene ring of the indole nucleus is planar. Slight deviations from planarity occur at the intersection of the benzene and heterocyclic rings, *e.g.* C(3)—C(4)—C(5)—C(6) and C(3)—C(4)—C(9)—N(1). However, there is considerable distortion in the heterocyclic part of the molecule as can be seen from the C(4)—C(9)—N(1)—C(2), C(9)—N(1)—C(2)—C(3), N(1)—C(2)—C(3)—O(3) and N(1)—C(2)—C(3)—C(4) torsion angles. The disposition of substituents on the heterocycle reflects both the hybridization state of N(1) and C(2) and also the non-planarity of the ring: C(3)—C(2)—N(1)—C(10) is antiperiplanar but appreciably different from 180°, while C(17)—C(2)—C(3)—C(4) and C(24)—C(2)—C(3)—C(4) are both anticlinal but 36° different in magnitude. Thus the C(10)···C(17) contact at 2·947 (3) Å is shorter than C(10)—C(24) [3·210 (3) Å].

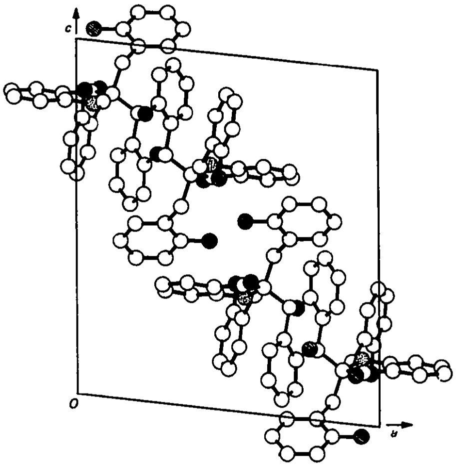

Fig. 2. Packing of molecules viewed down the *b* axis. Hydrogen atoms have been omitted for clarity; nitrogen atoms are stippled and oxygen atoms are hatched.

Rotations about the two single bonds linking each aromatic substituent to the indole system serve to keep the substituents well separated. Torsion angles about the exit bonds C(2)—N(1)—C(10)—C(11) and N(1)—C(2)—C(17)—C(18) are antiperiplanar, so that the C(11)···C(18) distance enlarges to 5·913 (4) Å. The remaining exit bond has N(1)—C(2)—C(24)—C(25) and C(3)—C(2)—C(24)—C(25) both synclinal, producing shorter but still unhindered C(11)···C(25) and C(18)···C(25) distances of 4·417 (4) and 4·633 (4) Å respectively. Torsion angles about the link bonds to the benzene rings are all synclinal or anticlinal.

The C—O bond lengths in the phenolic rings are 1·372 (3) Å for C(12)—O(12), 1·360 (3) Å for C(19)—O(19) and 1·362 (3) Å for C(26)—O(26), which may be expected for an O attached to an aromatic ring (*International Tables for X-ray Crystallography*, 1968). Torsion angles indicate that the phenolic rings are planar although the hydroxyl groups bend out of the planes, probably for intermolecular hydrogen bonding.

The molecules in the unit cell (Fig. 2) are linked twice in the **b** direction by hydrogen bonds both involving O(3) as proton acceptor: once from O(12) in a corresponding molecule in the adjacent unit cell [O···O distance 2·676 (3) Å] and once from O(26) in a molecule related by the screw axis [2·709 (3) Å]. Paired O(19)—H···O(12) interactions in centrosymmetrically related molecules [2·768 (3) Å] complete the network of hydrogen bonds and create a van der Waals contact of 2·952 (3) Å between O(19) and O(3).

Computations were carried out at the University of Manchester Regional Computing Centre.

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