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4-(1-Phenylethyl)benzene-1,3-diol

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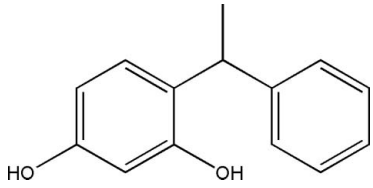
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.103; data-to-parameter ratio = 8.7.

There are two crystallographically independent molecules of the title compound, $C_{14}H_{14}O_2$, in the asymmetric unit. Intermolecular O—H···O hydrogen bonding between hydroxy groups occurs in the crystal structure, resulting in a supramolecular structure.

Related literature

For general background, see: Buu-Hoi *et al.* (1952).



Experimental

Crystal data

$C_{14}H_{14}O_2$
M_r = 214.25
Orthorhombic, $Pca2_1$
a = 13.131 (4) Å
b = 5.7841 (15) Å
c = 30.046 (8) Å
V = 2282.0 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.47 × 0.41 × 0.36 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: none
10800 measured reflections
2536 independent reflections
1675 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.103
S = 1.03
2536 reflections
293 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O4^{i}	0.82	1.94	2.745 (3)	166
O3—H3···O2	0.82	1.98	2.797 (3)	177
O4—H4···O1^{ii}	0.82	2.00	2.816 (3)	170

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2265).

References

Bruker (1999). *SMART* (Version 5.054), *SAINT-Plus* (Version 6.45) and *SHELXTL* (Version 6.14). Bruker AXS Inc, Madison, Wisconsin, USA.
Buu-Hoi, N. P., Le, B. H. & Binon, F. (1952). *J. Org. Chem.* **17**, 243–248.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

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4-(1-Phenylethyl)benzene-1,3-diol

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Comment

4-(1-Phenylethyl)benzene-1,3-diol is a polyphenol, which exhibits potential free radical scavenging property applied to food as antioxidant and potential tyrosinase inhibitory property applied to cosmetics as skin brightener (Buu-Hoi, *et al.*, 1952). We here report its crystal structure.

The X-ray study of the title compound confirms the previously proposed molecular structure based on spectroscopic data. There are two crystallographically independent molecules in the asymmetric unit (Fig. 1). Intermolecular O—H···O hydrogen bonding between hydroxy groups occurs in the crystal (Table 1), resulting in the supra-molecular structure (Fig. 2).

Experimental

Mixing 5.2 g styrene (0.05 mol) in 100 ml toluene with 11 g (0.1 mol) *m*-dihydroxybenzene and 1 g H_2SO_4 (0.01 mol) and refluxing the mixture for 6 h to give 8.6 g 4-(1-Phenylethyl)benzene-1,3-diol crystals after distilling and cooling the mixture to room temperature.

Refinement

H atoms bonded to O atoms were located in a difference map and refined with distance restraints of O—H = 0.82 Å, and with U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.98 Å and with U_{iso}(H) = 1.5U_{eq}(C) for methyl and 1.2U_{eq}(C) for others. In the absence of significant anomalous dispersion effects, Friedel pairs were merged.

Figures

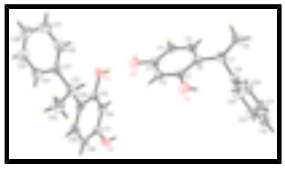

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

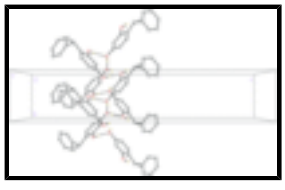

Fig. 2. The packing of (I), viewed down the *c* axis, showing one layer of molecules connected by O—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

4-(1-Phenylethyl)benzene-1,3-diol

Crystal data

$C_{14}H_{14}O_2$	F_{000} = 912
M_r = 214.25	D_x = 1.247 Mg m^{-3}
Orthorhombic, *Pca*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 984 reflections
a = 13.131 (4) Å	θ = 2.7–23.9º
b = 5.7841 (15) Å	μ = 0.08 mm^{-1}
c = 30.046 (8) Å	*T* = 293 (2) K
V = 2282.0 (10) Å^3	Block, colourless
Z = 8	0.47 × 0.41 × 0.36 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1675 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.035
Monochromator: graphite	θ_{max} = 27.1º
T = 293(2) K	θ_{min} = 3.1º
φ and ω scans	*h* = −16→16
Absorption correction: none	*k* = −7→5
10800 measured reflections	*l* = −38→36
2536 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.0955P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.103	$(\Delta/\sigma)_{max} < 0.001$
S = 1.03	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
2536 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
293 parameters	Extinction correction: none
1 restraint	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Special details

Experimental. The compound identity was conformed by the ^{1}H NMR spectra and ESI-MS. ^{1}H NMR (300 MHz, DMSO-d_6): δ 9.11(br, 1H, –OH), 8.98(br, 1H, –OH), 7.20–7.15 (5*H*, aromatic),7.10 (1*H*, aromatic), 6.82 (1*H*, aromatic), 6.22 (1*H*, aromatic), 6.14 (1*H*, aromatic) 4.30 (q, 1H), 1.44 (d, 3H). ESI-MS (m/*z*): 213$[M]^-$.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3184 (2)	0.1413 (5)	0.40687 (9)	0.0505 (7)
C2	0.3112 (2)	0.3209 (6)	0.37688 (10)	0.0524 (7)
H2A	0.3673	0.3616	0.3597	0.063*
C3	0.2211 (2)	0.4400 (6)	0.37243 (10)	0.0489 (7)
C4	0.1393 (2)	0.3845 (6)	0.39909 (11)	0.0564 (8)
H4A	0.0786	0.4664	0.3969	0.068*
C5	0.1493 (2)	0.2054 (6)	0.42905 (10)	0.0570 (8)
H5A	0.0938	0.1698	0.4470	0.068*
C6	0.2371 (2)	0.0756 (5)	0.43391 (9)	0.0477 (7)
C7	0.2454 (3)	−0.1395 (5)	0.46271 (10)	0.0544 (8)
H7A	0.2615	−0.2680	0.4426	0.065*
C8	0.1456 (3)	−0.2039 (7)	0.48646 (13)	0.0777 (11)
H8A	0.1560	−0.3404	0.5040	0.117*
H8B	0.0935	−0.2326	0.4647	0.117*
H8C	0.1250	−0.0788	0.5054	0.117*
C9	0.3289 (2)	−0.1328 (5)	0.49728 (10)	0.0506 (7)
C10	0.3943 (3)	−0.3191 (6)	0.50251 (12)	0.0711 (10)
H10A	0.3902	−0.4432	0.4829	0.085*
C11	0.4648 (3)	−0.3232 (7)	0.53610 (14)	0.0801 (11)
H11A	0.5069	−0.4514	0.5394	0.096*
C12	0.4742 (3)	−0.1426 (7)	0.56472 (12)	0.0744 (10)
H12A	0.5221	−0.1470	0.5875	0.089*
C13	0.4121 (3)	0.0462 (7)	0.55966 (13)	0.0716 (10)
H13A	0.4186	0.1718	0.5788	0.086*
C14	0.3395 (3)	0.0502 (6)	0.52595 (12)	0.0617 (9)
H14A	0.2975	0.1787	0.5228	0.074*
O1	0.40876 (18)	0.0228 (5)	0.40921 (8)	0.0709 (7)
H1	0.4109	−0.0510	0.4325	0.106*
O2	0.21656 (15)	0.6154 (4)	0.34190 (8)	0.0638 (6)

H2	0.1634	0.6879	0.3453	0.096*
C15	0.4370 (2)	0.6411 (6)	0.27380 (9)	0.0532 (8)
C16	0.4458 (2)	0.8177 (6)	0.30385 (9)	0.0533 (8)
H16A	0.3904	0.8601	0.3213	0.064*
C17	0.5374 (2)	0.9326 (6)	0.30808 (10)	0.0505 (7)
C18	0.6188 (2)	0.8732 (6)	0.28212 (11)	0.0552 (8)
H18A	0.6804	0.9513	0.2848	0.066*
C19	0.6079 (2)	0.6948 (6)	0.25181 (11)	0.0568 (8)
H19A	0.6630	0.6568	0.2338	0.068*
C20	0.5186 (2)	0.5709 (5)	0.24720 (9)	0.0490 (7)
C21	0.5059 (2)	0.3644 (5)	0.21609 (11)	0.0570 (8)
H21A	0.4821	0.2352	0.2344	0.068*
C22	0.6056 (3)	0.2857 (7)	0.19424 (13)	0.0758 (10)
H22A	0.6558	0.2579	0.2168	0.114*
H22B	0.6295	0.4041	0.1744	0.114*
H22C	0.5939	0.1460	0.1778	0.114*
C23	0.4250 (2)	0.4040 (5)	0.18056 (11)	0.0517 (8)
C24	0.4247 (3)	0.6009 (6)	0.15445 (11)	0.0609 (8)
H24A	0.4724	0.7165	0.1598	0.073*
C25	0.3549 (3)	0.6287 (7)	0.12061 (12)	0.0709 (9)
H25A	0.3559	0.7627	0.1035	0.085*
C26	0.2847 (3)	0.4624 (7)	0.11196 (13)	0.0740 (10)
H26A	0.2378	0.4819	0.0890	0.089*
C27	0.2834 (3)	0.2660 (7)	0.13724 (14)	0.0759 (10)
H27A	0.2356	0.1513	0.1314	0.091*
C28	0.3524 (3)	0.2367 (6)	0.17134 (12)	0.0650 (9)
H28A	0.3503	0.1026	0.1884	0.078*
O3	0.34586 (18)	0.5241 (5)	0.27004 (9)	0.0731 (7)
H3	0.3095	0.5549	0.2914	0.110*
O4	0.54612 (17)	1.1101 (4)	0.33921 (8)	0.0672 (6)
H4	0.5120	1.0786	0.3612	0.101*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0398 (16)	0.0738 (19)	0.0378 (16)	0.0007 (14)	0.0008 (12)	−0.0042 (15)
C2	0.0360 (15)	0.079 (2)	0.0419 (15)	0.0021 (14)	0.0078 (12)	0.0001 (16)
C3	0.0410 (17)	0.0643 (19)	0.0413 (17)	0.0004 (14)	0.0024 (14)	−0.0099 (15)
C4	0.0353 (16)	0.076 (2)	0.0575 (19)	0.0010 (15)	0.0050 (14)	−0.0120 (18)
C5	0.0408 (17)	0.077 (2)	0.0534 (18)	−0.0125 (15)	0.0118 (14)	−0.0090 (17)
C6	0.0414 (16)	0.0636 (17)	0.0381 (16)	−0.0067 (15)	0.0056 (13)	−0.0104 (14)
C7	0.0554 (18)	0.0586 (18)	0.0492 (18)	−0.0098 (15)	0.0112 (14)	−0.0140 (14)
C8	0.068 (2)	0.090 (3)	0.076 (2)	−0.0267 (19)	0.0135 (19)	0.005 (2)
C9	0.0533 (18)	0.0514 (17)	0.0471 (18)	−0.0020 (14)	0.0142 (14)	−0.0005 (14)
C10	0.086 (3)	0.059 (2)	0.068 (2)	0.0082 (19)	0.019 (2)	0.0012 (17)
C11	0.079 (3)	0.076 (2)	0.085 (3)	0.023 (2)	0.011 (2)	0.020 (2)
C12	0.057 (2)	0.100 (3)	0.066 (2)	0.005 (2)	−0.0010 (18)	0.022 (2)
C13	0.070 (2)	0.081 (3)	0.064 (2)	0.003 (2)	−0.0053 (19)	−0.0122 (19)

C14	0.063 (2)	0.062 (2)	0.060 (2)	0.0120 (16)	0.0007 (17)	−0.0068 (17)
O1	0.0482 (14)	0.1065 (19)	0.0579 (18)	0.0221 (12)	0.0097 (12)	0.0169 (13)
O2	0.0518 (14)	0.0757 (15)	0.0637 (15)	0.0183 (11)	0.0078 (11)	0.0049 (12)
C15	0.0384 (16)	0.082 (2)	0.0394 (16)	−0.0084 (14)	0.0028 (12)	0.0044 (15)
C16	0.0396 (17)	0.079 (2)	0.0412 (16)	−0.0064 (14)	0.0066 (13)	−0.0025 (16)
C17	0.0455 (18)	0.065 (2)	0.0413 (17)	−0.0060 (15)	−0.0003 (14)	0.0051 (15)
C18	0.0360 (16)	0.071 (2)	0.0588 (19)	−0.0060 (15)	0.0036 (14)	0.0058 (17)
C19	0.0405 (17)	0.071 (2)	0.0585 (19)	0.0054 (15)	0.0110 (14)	0.0090 (17)
C20	0.0410 (17)	0.0626 (19)	0.0435 (17)	0.0050 (15)	0.0035 (13)	0.0066 (14)
C21	0.0609 (19)	0.0572 (18)	0.0530 (19)	0.0029 (16)	0.0110 (17)	0.0069 (15)
C22	0.068 (2)	0.081 (2)	0.078 (2)	0.0172 (18)	0.0145 (19)	−0.004 (2)
C23	0.0540 (19)	0.0550 (18)	0.0461 (17)	0.0007 (15)	0.0126 (14)	−0.0056 (14)
C24	0.068 (2)	0.0565 (19)	0.058 (2)	−0.0060 (16)	−0.0018 (17)	0.0010 (16)
C25	0.084 (3)	0.071 (2)	0.058 (2)	0.008 (2)	−0.0048 (19)	−0.0001 (18)
C26	0.063 (2)	0.090 (3)	0.069 (2)	0.008 (2)	−0.0070 (19)	−0.018 (2)
C27	0.059 (2)	0.082 (3)	0.086 (3)	−0.0068 (19)	−0.001 (2)	−0.020 (2)
C28	0.064 (2)	0.0587 (19)	0.072 (2)	−0.0054 (16)	0.0144 (18)	−0.0040 (17)
O3	0.0437 (13)	0.119 (2)	0.0565 (16)	−0.0240 (13)	0.0128 (12)	−0.0153 (13)
O4	0.0624 (14)	0.0819 (16)	0.0573 (15)	−0.0196 (12)	0.0141 (11)	−0.0042 (12)

Geometric parameters (Å, °)

C1—O1	1.372 (4)	C15—C16	1.369 (4)
C1—C2	1.378 (4)	C15—O3	1.379 (4)
C1—C6	1.395 (4)	C15—C20	1.398 (4)
C2—C3	1.375 (4)	C16—C17	1.381 (4)
C2—H2A	0.9300	C16—H16A	0.9300
C3—O2	1.369 (4)	C17—C18	1.367 (4)
C3—C4	1.378 (4)	C17—O4	1.393 (4)
C4—C5	1.379 (5)	C18—C19	1.384 (5)
C4—H4A	0.9300	C18—H18A	0.9300
C5—C6	1.384 (4)	C19—C20	1.381 (5)
C5—H5A	0.9300	C19—H19A	0.9300
C6—C7	1.519 (4)	C20—C21	1.526 (4)
C7—C9	1.510 (5)	C21—C23	1.523 (5)
C7—C8	1.538 (5)	C21—C22	1.534 (5)
C7—H7A	0.9800	C21—H21A	0.9800
C8—H8A	0.9600	C22—H22A	0.9600
C8—H8B	0.9600	C22—H22B	0.9600
C8—H8C	0.9600	C22—H22C	0.9600
C9—C14	1.372 (5)	C23—C24	1.383 (4)
C9—C10	1.387 (5)	C23—C28	1.386 (5)
C10—C11	1.370 (6)	C24—C25	1.378 (5)
C10—H10A	0.9300	C24—H24A	0.9300
C11—C12	1.358 (5)	C25—C26	1.358 (5)
C11—H11A	0.9300	C25—H25A	0.9300
C12—C13	1.371 (5)	C26—C27	1.367 (5)
C12—H12A	0.9300	C26—H26A	0.9300
C13—C14	1.391 (5)	C27—C28	1.379 (5)

C13—H13A	0.9300	C27—H27A	0.9300
C14—H14A	0.9300	C28—H28A	0.9300
O1—H1	0.8200	O3—H3	0.8200
O2—H2	0.8200	O4—H4	0.8200
O1—C1—C2	118.0 (3)	C16—C15—O3	119.6 (3)
O1—C1—C6	119.7 (3)	C16—C15—C20	122.0 (3)
C2—C1—C6	122.3 (3)	O3—C15—C20	118.4 (3)
C3—C2—C1	120.0 (3)	C15—C16—C17	119.6 (3)
C3—C2—H2A	120.0	C15—C16—H16A	120.2
C1—C2—H2A	120.0	C17—C16—H16A	120.2
O2—C3—C2	118.3 (3)	C18—C17—C16	120.5 (3)
O2—C3—C4	121.9 (3)	C18—C17—O4	120.3 (3)
C2—C3—C4	119.8 (3)	C16—C17—O4	119.2 (3)
C3—C4—C5	118.7 (3)	C17—C18—C19	118.8 (3)
C3—C4—H4A	120.6	C17—C18—H18A	120.6
C5—C4—H4A	120.6	C19—C18—H18A	120.6
C4—C5—C6	123.8 (3)	C20—C19—C18	122.8 (3)
C4—C5—H5A	118.1	C20—C19—H19A	118.6
C6—C5—H5A	118.1	C18—C19—H19A	118.6
C5—C6—C1	115.4 (3)	C19—C20—C15	116.3 (3)
C5—C6—C7	124.4 (3)	C19—C20—C21	124.1 (3)
C1—C6—C7	120.0 (3)	C15—C20—C21	119.6 (3)
C9—C7—C6	115.0 (3)	C23—C21—C20	112.9 (2)
C9—C7—C8	107.8 (3)	C23—C21—C22	109.9 (3)
C6—C7—C8	113.6 (3)	C20—C21—C22	113.6 (3)
C9—C7—H7A	106.6	C23—C21—H21A	106.7
C6—C7—H7A	106.6	C20—C21—H21A	106.7
C8—C7—H7A	106.6	C22—C21—H21A	106.7
C7—C8—H8A	109.5	C21—C22—H22A	109.5
C7—C8—H8B	109.5	C21—C22—H22B	109.5
H8A—C8—H8B	109.5	H22A—C22—H22B	109.5
C7—C8—H8C	109.5	C21—C22—H22C	109.5
H8A—C8—H8C	109.5	H22A—C22—H22C	109.5
H8B—C8—H8C	109.5	H22B—C22—H22C	109.5
C14—C9—C10	117.8 (3)	C24—C23—C28	117.3 (3)
C14—C9—C7	121.7 (3)	C24—C23—C21	121.6 (3)
C10—C9—C7	120.5 (3)	C28—C23—C21	121.0 (3)
C11—C10—C9	121.0 (4)	C25—C24—C23	121.1 (3)
C11—C10—H10A	119.5	C25—C24—H24A	119.4
C9—C10—H10A	119.5	C23—C24—H24A	119.4
C12—C11—C10	120.9 (3)	C26—C25—C24	120.7 (3)
C12—C11—H11A	119.5	C26—C25—H25A	119.7
C10—C11—H11A	119.5	C24—C25—H25A	119.7
C11—C12—C13	119.2 (4)	C25—C26—C27	119.4 (4)
C11—C12—H12A	120.4	C25—C26—H26A	120.3
C13—C12—H12A	120.4	C27—C26—H26A	120.3
C12—C13—C14	120.1 (4)	C26—C27—C28	120.5 (3)
C12—C13—H13A	119.9	C26—C27—H27A	119.8
C14—C13—H13A	119.9	C28—C27—H27A	119.8

C9—C14—C13	120.9 (3)	C27—C28—C23	121.0 (3)
C9—C14—H14A	119.5	C27—C28—H28A	119.5
C13—C14—H14A	119.5	C23—C28—H28A	119.5
C1—O1—H1	109.5	C15—O3—H3	109.5
C3—O2—H2	109.5	C17—O4—H4	109.5
O1—C1—C2—C3	178.0 (3)	O3—C15—C16—C17	179.1 (3)
C6—C1—C2—C3	−0.9 (4)	C20—C15—C16—C17	0.6 (5)
C1—C2—C3—O2	−179.2 (3)	C15—C16—C17—C18	0.8 (5)
C1—C2—C3—C4	2.3 (4)	C15—C16—C17—O4	−179.1 (3)
O2—C3—C4—C5	179.9 (3)	C16—C17—C18—C19	−0.5 (5)
C2—C3—C4—C5	−1.6 (5)	O4—C17—C18—C19	179.4 (3)
C3—C4—C5—C6	−0.4 (5)	C17—C18—C19—C20	−1.2 (5)
C4—C5—C6—C1	1.6 (4)	C18—C19—C20—C15	2.5 (5)
C4—C5—C6—C7	−172.5 (3)	C18—C19—C20—C21	−176.3 (3)
O1—C1—C6—C5	−179.9 (3)	C16—C15—C20—C19	−2.2 (4)
C2—C1—C6—C5	−1.0 (4)	O3—C15—C20—C19	179.3 (3)
O1—C1—C6—C7	−5.5 (4)	C16—C15—C20—C21	176.7 (3)
C2—C1—C6—C7	173.4 (3)	O3—C15—C20—C21	−1.8 (4)
C5—C6—C7—C9	−124.6 (3)	C19—C20—C21—C23	−118.7 (3)
C1—C6—C7—C9	61.6 (4)	C15—C20—C21—C23	62.6 (4)
C5—C6—C7—C8	0.4 (4)	C19—C20—C21—C22	7.3 (4)
C1—C6—C7—C8	−173.5 (3)	C15—C20—C21—C22	−171.5 (3)
C6—C7—C9—C14	50.6 (4)	C20—C21—C23—C24	50.4 (4)
C8—C7—C9—C14	−77.3 (4)	C22—C21—C23—C24	−77.5 (4)
C6—C7—C9—C10	−132.8 (3)	C20—C21—C23—C28	−133.5 (3)
C8—C7—C9—C10	99.3 (3)	C22—C21—C23—C28	98.5 (3)
C14—C9—C10—C11	2.1 (5)	C28—C23—C24—C25	−0.1 (5)
C7—C9—C10—C11	−174.6 (3)	C21—C23—C24—C25	176.1 (3)
C9—C10—C11—C12	−1.4 (6)	C23—C24—C25—C26	−0.2 (5)
C10—C11—C12—C13	−0.2 (6)	C24—C25—C26—C27	0.1 (5)
C11—C12—C13—C14	1.0 (5)	C25—C26—C27—C28	0.2 (5)
C10—C9—C14—C13	−1.3 (5)	C26—C27—C28—C23	−0.5 (5)
C7—C9—C14—C13	175.3 (3)	C24—C23—C28—C27	0.4 (5)
C12—C13—C14—C9	−0.2 (5)	C21—C23—C28—C27	−175.7 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O4^{i}	0.82	1.94	2.745 (3)	166
O3—H3···O2	0.82	1.98	2.797 (3)	177
O4—H4···O1^{ii}	0.82	2.00	2.816 (3)	170

Symmetry codes: (i) *x*−1/2, −*y*+2, *z*; (ii) *x*, *y*+1, *z*.

Fig. 1

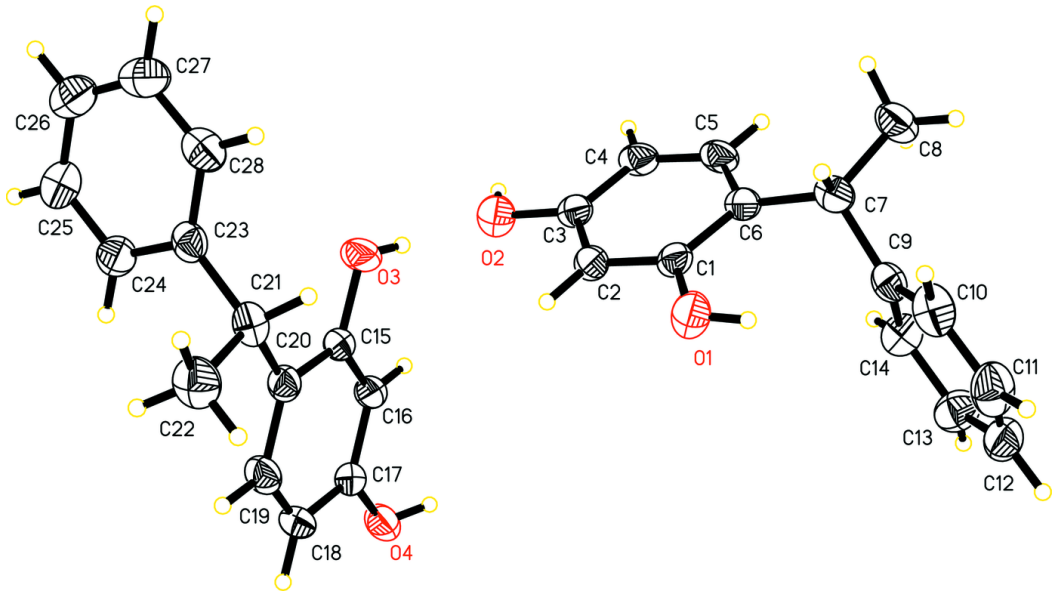
C27
C26
C28
C25
C23
C24
C21
O3
C20
C15
C22
C16
C17
C19
C18
O4
C5
C4
C8
C7
O2
C3
C6
C9
C1
C2
C10
O1
C14
C11
C13
C12

Fig. 2