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(*E*)-1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one monohydrate

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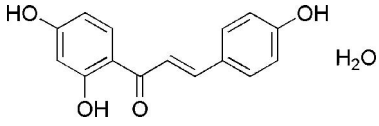
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.057; wR factor = 0.144; data-to-parameter ratio = 13.4.

In the title compound, $C_{15}H_{12}O_4\cdot H_2O$, the two benzene rings are not coplanar, making a dihedral angle of 7.24 (16)°. An intramolecular hydroxy–carbonyl O—H···O hydrogen bond occurs. In the crystal, four intermolecular O—H···O hydrogen bonds involving the hydroxy residues, the carbonyl group and the water molecule lead to the formation of a three-dimensional network. The supramolecular structure is further stabilized by weak C—H···O interactions.

Related literature

For the biological activity of the title compound, see: Jang *et al.* (2008); Liu *et al.* (2008). For a related structure, see: Ma *et al.* (2005).



Experimental

Crystal data

$C_{15}H_{12}O_4\cdot H_2O$
M_r = 274.26
Monoclinic, $P2_1/c$
a = 11.489 (2) Å
b = 9.5903 (17) Å
c = 12.498 (2) Å
β = 103.649 (3)°
V = 1338.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.12 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.988, T_{max} = 0.990
8297 measured reflections
2625 independent reflections
2115 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.144
S = 1.09
2625 reflections
196 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O3	0.87 (2)	1.74 (2)	2.530 (2)	150 (3)
O2—H2A···O5^{i}	0.82 (2)	1.83 (2)	2.644 (3)	175 (4)
O4—H4A···O3^{ii}	0.83 (2)	1.95 (2)	2.776 (2)	175 (4)
O5—H5A···O1^{iii}	0.84 (2)	1.99 (2)	2.802 (2)	164 (3)
O5—H5B···O4^{iv}	0.84 (2)	1.97 (2)	2.785 (3)	165 (3)
C9—H9···O4^{v}	0.93	2.56	3.402 (3)	151

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z-\frac{1}{2}$; (iii) $-x, -y+2, -z$; (iv) $-x+1, -y+1, -z$; (v) $-x+1, y+\frac{1}{2}, -z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: GO2004).

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Liu, B., Yang, J., Wen, Q. S. & Li, Y. (2008). *Eur. J. Pharmacol.* **587**, 257–266
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supporting information

Acta Cryst. (2011). E**67**, o732 [doi:10.1107/S1600536811006271]

(*E*)-1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one monohydrate

Jian-Guo Wang, Lin Wu, Chan-Juan Zhong, Zhao-Hui Ouyang and De-Lian Yi

S1. Comment

The title compound exhibits many biological activities such as tracheal relaxation effects (Liu *et al.*, 2008) and suppressing cocaine-induced extracellular dopamine release (Jang *et al.*, 2008).

One (*E*)-1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one molecule bears one crystalline water molecule (Fig.1). In the molecule, the two benzene rings are not coplanar, the dihedral angle being 7.24 (16)°. The structure displays O—H···O and C—H···O hydrogen bonding (Table 1 and Fig. 2).

S2. Experimental

2, 4-dihydroxyacetophenone (7.6 g, 0.05 mol) and 4-hydroxybenzaldehyde (8.54 g, 0.07 mol) were dissolved in diglycol (25 ml). Then 40% aq. KOH (50 ml) was added, and the reaction mixture was vigorously stirred under nitrogen atmosphere at 333 K for 2 h. The progress of the reaction was monitored by thin- layer chromatography (Si gel, developing solvent *V*(ethyl acetate)/*V*(benzene) = 1:2). The mixture was colled to room temperature and 1:1 (*v*/*v*) hydrochloric acid was added to acidize the mixture to pH=3 and a solid was obtained. After crystallized by ethanol-water, crystalline yellow needles were obtained, m.p. 472.5–474.2 K.

S3. Refinement

All the carbon-bounded hydrogen atoms were located at their ideal positions with the C—H=0.93Å and U_{iso}(H)=1.2U_{eq}(C). All the hydrogen atoms bonded to the oxygen atoms were located from the difference maps and refined with the restraints of O—H=0.82 (1)Å and U_{iso}(H)=1.5U_{eq}(O).

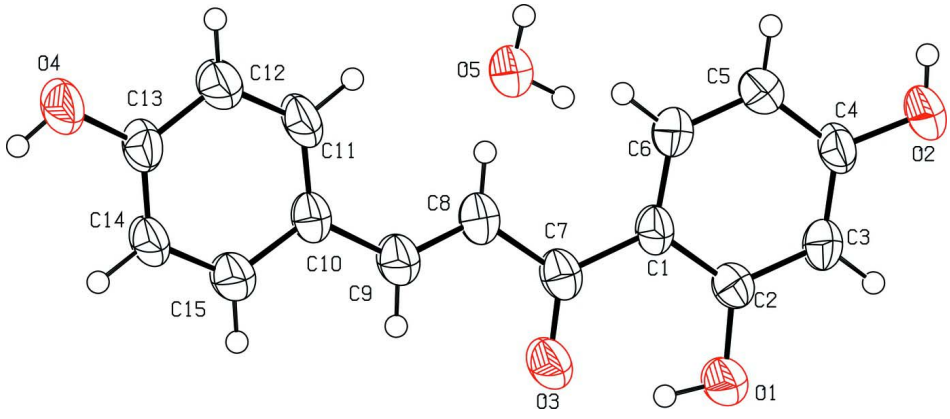

Figure 1

View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

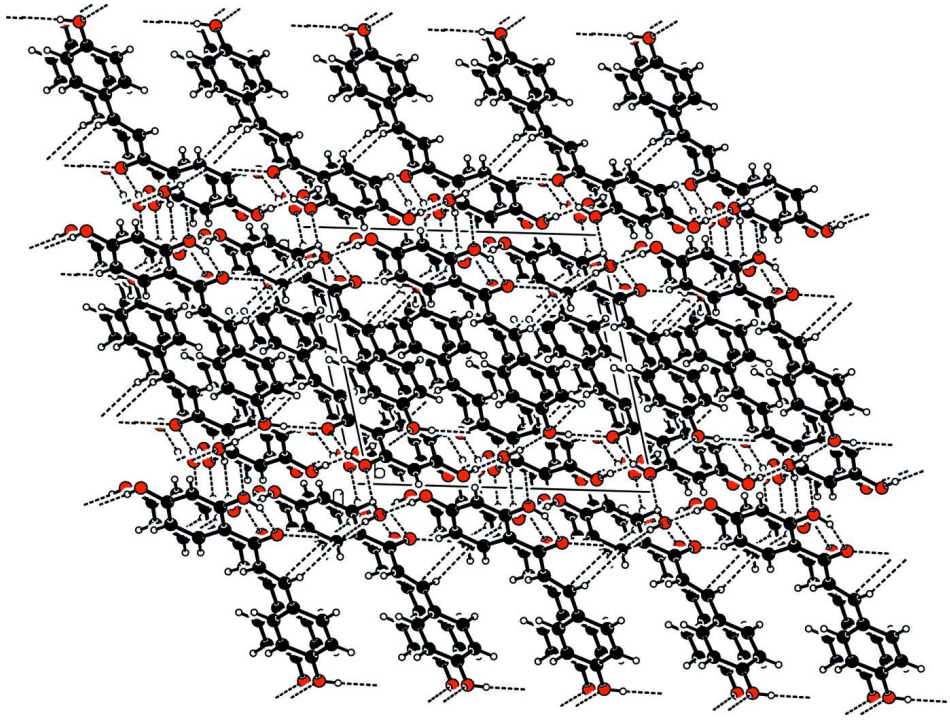

Figure 2

The crystal packing for (I), with O—H···O and C—H···O interactions shown as dashed lines.

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$\beta = 103.649\ (3)°$
$V = 1338.2\ (4)$ Å^3
$Z = 4$
$F(000) = 576$
$D_x = 1.361$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2288 reflections
$\theta = 2.7–25.3°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, yellow
0.12 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.988$, $T_{max} = 0.990$
8297 measured reflections
2625 independent reflections
2115 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.7°$
$h = -14 \rightarrow 14$
$k = -11 \rightarrow 9$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.144$
$S = 1.09$
2625 reflections
196 parameters
5 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.499P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.19653 (18)	1.0001 (2)	0.07068 (17)	0.0402 (5)
C2	0.10947 (18)	1.1026 (2)	0.07420 (17)	0.0412 (5)
C3	0.0605 (2)	1.1156 (2)	0.16459 (19)	0.0475 (6)
H3	0.0037	1.1844	0.1655	0.057*
C4	0.0950 (2)	1.0275 (2)	0.25329 (18)	0.0452 (5)
C5	0.1818 (2)	0.9256 (3)	0.25306 (19)	0.0500 (6)
H5	0.2061	0.8663	0.3131	0.060*
C6	0.2309 (2)	0.9138 (2)	0.16359 (19)	0.0473 (6)
H6	0.2892	0.8462	0.1644	0.057*
C7	0.24678 (19)	0.9881 (2)	−0.02538 (18)	0.0437 (5)
C8	0.3403 (2)	0.8856 (3)	−0.02910 (19)	0.0494 (6)
H8	0.3588	0.8183	0.0258	0.059*
C9	0.3990 (2)	0.8858 (3)	−0.10772 (19)	0.0493 (6)
H9	0.3751	0.9540	−0.1613	0.059*
C10	0.49523 (19)	0.7959 (2)	−0.12387 (17)	0.0431 (5)
C11	0.5467 (2)	0.6925 (3)	−0.05077 (19)	0.0566 (7)
H11	0.5169	0.6760	0.0111	0.068*
C12	0.6406 (2)	0.6134 (3)	−0.0672 (2)	0.0635 (7)
H12	0.6750	0.5458	−0.0161	0.076*
C13	0.68407 (19)	0.6350 (3)	−0.16102 (18)	0.0474 (6)
C14	0.6341 (2)	0.7353 (3)	−0.23509 (18)	0.0486 (6)
H14	0.6628	0.7498	−0.2978	0.058*
C15	0.5412 (2)	0.8148 (3)	−0.21662 (19)	0.0518 (6)
H15	0.5080	0.8832	−0.2675	0.062*

O1	0.07099 (15)	1.19360 (19)	−0.01001 (14)	0.0589 (5)
H1A	0.107 (3)	1.171 (3)	−0.061 (2)	0.088*
O2	0.04269 (18)	1.0443 (2)	0.33756 (14)	0.0649 (5)
H2A	0.069 (3)	0.988 (3)	0.387 (2)	0.097*
O3	0.21067 (14)	1.06876 (19)	−0.10709 (13)	0.0565 (5)
O4	0.77775 (17)	0.5545 (2)	−0.17385 (14)	0.0668 (6)
H4A	0.784 (3)	0.563 (4)	−0.2384 (17)	0.100*
O5	0.12061 (17)	0.6281 (2)	0.00416 (14)	0.0587 (5)
H5A	0.072 (2)	0.687 (3)	0.017 (3)	0.088*
H5B	0.149 (3)	0.586 (3)	0.0630 (19)	0.088*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0381 (11)	0.0444 (12)	0.0430 (12)	−0.0015 (9)	0.0192 (9)	−0.0060 (10)
C2	0.0413 (11)	0.0446 (12)	0.0415 (11)	−0.0002 (10)	0.0174 (9)	0.0015 (10)
C3	0.0457 (12)	0.0512 (14)	0.0524 (13)	0.0090 (11)	0.0251 (10)	−0.0011 (11)
C4	0.0502 (12)	0.0514 (13)	0.0409 (12)	0.0005 (10)	0.0247 (10)	−0.0039 (10)
C5	0.0583 (14)	0.0530 (14)	0.0436 (12)	0.0078 (11)	0.0217 (11)	0.0070 (10)
C6	0.0485 (12)	0.0485 (13)	0.0497 (13)	0.0086 (10)	0.0213 (10)	−0.0007 (10)
C7	0.0400 (11)	0.0520 (14)	0.0432 (12)	−0.0049 (10)	0.0183 (9)	−0.0041 (10)
C8	0.0513 (13)	0.0551 (14)	0.0483 (13)	0.0061 (11)	0.0249 (10)	−0.0017 (11)
C9	0.0475 (12)	0.0576 (15)	0.0485 (13)	0.0041 (11)	0.0229 (10)	0.0008 (11)
C10	0.0404 (11)	0.0506 (13)	0.0431 (12)	−0.0005 (10)	0.0193 (10)	−0.0044 (10)
C11	0.0605 (15)	0.0757 (18)	0.0437 (13)	0.0113 (13)	0.0323 (12)	0.0049 (12)
C12	0.0690 (16)	0.0791 (19)	0.0495 (14)	0.0290 (15)	0.0285 (12)	0.0156 (13)
C13	0.0425 (12)	0.0596 (15)	0.0446 (12)	0.0065 (11)	0.0193 (10)	−0.0039 (11)
C14	0.0493 (13)	0.0617 (15)	0.0427 (12)	0.0062 (11)	0.0267 (10)	0.0028 (11)
C15	0.0528 (13)	0.0586 (15)	0.0507 (14)	0.0097 (11)	0.0254 (11)	0.0083 (11)
O1	0.0648 (11)	0.0665 (12)	0.0538 (10)	0.0202 (9)	0.0307 (8)	0.0141 (9)
O2	0.0793 (13)	0.0756 (13)	0.0531 (10)	0.0183 (10)	0.0424 (10)	0.0072 (9)
O3	0.0571 (10)	0.0710 (12)	0.0492 (9)	0.0108 (8)	0.0284 (8)	0.0084 (8)
O4	0.0654 (11)	0.0920 (14)	0.0512 (10)	0.0355 (10)	0.0302 (9)	0.0110 (10)
O5	0.0702 (12)	0.0605 (12)	0.0539 (10)	0.0151 (9)	0.0315 (9)	0.0043 (9)

Geometric parameters (Å, º)

C1—C6	1.405 (3)	C9—H9	0.9300
C1—C2	1.410 (3)	C10—C11	1.383 (3)
C1—C7	1.454 (3)	C10—C15	1.394 (3)
C2—O1	1.359 (3)	C11—C12	1.374 (3)
C2—C3	1.382 (3)	C11—H11	0.9300
C3—C4	1.375 (3)	C12—C13	1.393 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—O2	1.340 (3)	C13—C14	1.364 (3)
C4—C5	1.397 (3)	C13—O4	1.364 (3)
C5—C6	1.371 (3)	C14—C15	1.375 (3)
C5—H5	0.9300	C14—H14	0.9300

C6—H6	0.9300	C15—H15	0.9300
C7—O3	1.270 (3)	O1—H1A	0.867 (18)
C7—C8	1.465 (3)	O2—H2A	0.819 (18)
C8—C9	1.316 (3)	O4—H4A	0.829 (18)
C8—H8	0.9300	O5—H5A	0.836 (18)
C9—C10	1.453 (3)	O5—H5B	0.836 (18)

C6—C1—C2	116.61 (18)	C8—C9—H9	115.0
C6—C1—C7	123.2 (2)	C10—C9—H9	115.0
C2—C1—C7	120.24 (19)	C11—C10—C15	117.1 (2)
O1—C2—C3	117.03 (19)	C11—C10—C9	123.66 (19)
O1—C2—C1	121.81 (18)	C15—C10—C9	119.2 (2)
C3—C2—C1	121.2 (2)	C12—C11—C10	121.7 (2)
C4—C3—C2	120.5 (2)	C12—C11—H11	119.1
C4—C3—H3	119.7	C10—C11—H11	119.1
C2—C3—H3	119.7	C11—C12—C13	119.6 (2)
O2—C4—C3	117.5 (2)	C11—C12—H12	120.2
O2—C4—C5	122.6 (2)	C13—C12—H12	120.2
C3—C4—C5	119.90 (19)	C14—C13—O4	122.43 (19)
C6—C5—C4	119.4 (2)	C14—C13—C12	119.9 (2)
C6—C5—H5	120.3	O4—C13—C12	117.6 (2)
C4—C5—H5	120.3	C13—C14—C15	119.7 (2)
C5—C6—C1	122.4 (2)	C13—C14—H14	120.1
C5—C6—H6	118.8	C15—C14—H14	120.1
C1—C6—H6	118.8	C14—C15—C10	121.9 (2)
O3—C7—C1	119.85 (19)	C14—C15—H15	119.0
O3—C7—C8	119.07 (19)	C10—C15—H15	119.0
C1—C7—C8	121.1 (2)	C2—O1—H1A	107 (2)
C9—C8—C7	122.1 (2)	C4—O2—H2A	111 (3)
C9—C8—H8	119.0	C13—O4—H4A	108 (2)
C7—C8—H8	119.0	H5A—O5—H5B	107 (3)
C8—C9—C10	130.0 (2)		

C6—C1—C2—O1	178.7 (2)	C2—C1—C7—C8	177.9 (2)
C7—C1—C2—O1	−0.9 (3)	O3—C7—C8—C9	8.8 (4)
C6—C1—C2—C3	−0.5 (3)	C1—C7—C8—C9	−170.2 (2)
C7—C1—C2—C3	179.9 (2)	C7—C8—C9—C10	178.4 (2)
O1—C2—C3—C4	−179.8 (2)	C8—C9—C10—C11	−3.0 (4)
C1—C2—C3—C4	−0.6 (3)	C8—C9—C10—C15	178.3 (3)
C2—C3—C4—O2	−179.0 (2)	C15—C10—C11—C12	1.3 (4)
C2—C3—C4—C5	1.1 (4)	C9—C10—C11—C12	−177.5 (2)
O2—C4—C5—C6	179.5 (2)	C10—C11—C12—C13	−1.5 (4)
C3—C4—C5—C6	−0.6 (4)	C11—C12—C13—C14	0.7 (4)
C4—C5—C6—C1	−0.5 (4)	C11—C12—C13—O4	179.7 (2)
C2—C1—C6—C5	1.1 (3)	O4—C13—C14—C15	−178.9 (2)
C7—C1—C6—C5	−179.4 (2)	C12—C13—C14—C15	0.1 (4)
C6—C1—C7—O3	179.3 (2)	C13—C14—C15—C10	−0.3 (4)
C2—C1—C7—O3	−1.1 (3)	C11—C10—C15—C14	−0.4 (4)

C6—C1—C7—C8	−1.7 (3)	C9—C10—C15—C14	178.4 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O3	0.87 (2)	1.74 (2)	2.530 (2)	150 (3)
O2—H2*A*···O5^{i}	0.82 (2)	1.83 (2)	2.644 (3)	175 (4)
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O5—H5*A*···O1^{iii}	0.84 (2)	1.99 (2)	2.802 (2)	164 (3)
O5—H5*B*···O4^{iv}	0.84 (2)	1.97 (2)	2.785 (3)	165 (3)
C9—H9···O4^{v}	0.93	2.56	3.402 (3)	151

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