Crystal structure of *E*-1-(phenyl)-3-(4-hydroxyphenyl)-2-propene-1-one, $C_{15}H_{12}O_2$

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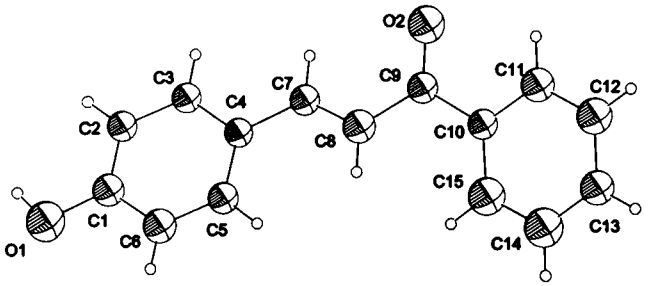

Abstract

$C_{15}H_{12}O_2$, orthorhombic, $P2_12_12_1$ (No. 19), $a = 5.3685(4)$ Å, $b = 12.957(2)$ Å, $c = 17.174(1)$ Å, $V = 1194.6$ Å^3, $Z = 4$, $R_{gt}(F) = 0.046$, $wR_{ref}(F^2) = 0.143$, $T = 293$ K.

Source of material

Transparent plate shaped crystals of the title compound were obtained from a solution of the compound in methanol by slow evaporation at room temperature.

Experimental details

The H atoms were allowed to ride on their parent atom with $U_{iso} = xU_{eq}$ (parent), where $x = 1.5$ for methyl and $x = 1.2$ for all others. The absolute structure was established by the Flack method [1], the Flack parameter for the inverted structure was found to be 0.2(5).

Discussion

This structural analysis was undertaken as part of continuing study of phenyl and hydroxyphenyl substituted 2-propene-1-one compounds [2-4]. The title compound is one of the intermediates used in the synthesis of mesogenic compound.

The conformation about the C7=C8 bond is *E* as found in the related compound as described in [2]. A least squares plane calculation suggests that the hydroxyphenyl ring A, C1/C2/C3/C4/C5/C6, makes an angle 8.5(2)° with respect to the plane defined by C7/C8/C9. The phenyl ring B, C10/C11/C12/C13/C14/C15 makes an angle 17.1(2)° with respect to the same plane. The dihedral angle between the planes of the rings A and B is 25.2(1)°. The group of atoms of the ring A deviates significantly from planarity with mean deviation –6.051(1) Å and for ring B it is –8.255(1) Å. This is also evident from the torsion angles ∠O1–C1–C2–C3 = 179.3(3)°, ∠O1–C1–C6–C5 = –180.0(3)°, ∠C9–C10–C11–C12 = 179.5(3)°, ∠C9–C10–C15–C14 = –178.9(3)°. The puckering parameters of the six membered rings have been calculated using the method of Cremer and Pople [5]. The phenyl ring B adopts boat conformation with q_3=0 and q_2=Q. The hydroxyphenyl ring A is in a half-chair conformation distorted towards a half-boat as described in [6]. The puckering parameters are included in the deposit CIF. Bond lengths observed here are clearly compatible with the proposed structure of the title compound and in particular the double bond character of the C7—C8 bond and the phenolic nature of O1. The length of the molecule in the crystalline state is found to be 11.26 Å. In the title compound, two intramolecular C–H···O interactions together with van der Waals interactions stabilize the molecular and packing structures in the crystal.

Table 1. Data collection and handling.

Crystal:	colourless plate, size 0.40 × 0.30 × 0.25 mm
Wavelength:	Cu K_α radiation (1.54180 Å)
μ:	6.58 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius-CAD4, $\omega/2\theta$
$2\theta_{max}$:	149.36°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1873, 1718
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1411
$N(param)_{refined}$:	156
Programs:	SHELXS-97 [7], SHELXL-97 [8], SHELXTL-plus [9], ZORTEP [10], PLATON [11]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	4*a*	–0.0157	0.4915	0.4781	0.088
H(3)	4*a*	0.0923	0.5031	0.6074	0.088
H(5)	4*a*	0.6709	0.6829	0.5506	0.087
H(6)	4*a*	0.5670	0.6688	0.4221	0.094
H(7)	4*a*	0.3697	0.5564	0.7099	0.082
H(8)	4*a*	0.7574	0.6860	0.6754	0.085
H(11)	4*a*	0.9802	0.6194	0.9191	0.090
H(12)	4*a*	1.2927	0.7180	0.9715	0.104
H(13)	4*a*	1.4466	0.8580	0.9033	0.106
H(14)	4*a*	1.2784	0.9005	0.7846	0.105
H(15)	4*a*	0.9591	0.8034	0.7326	0.091
H(16)	4*a*	0.1071	0.5303	0.3515	0.146

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*a*	0.2633(6)	0.5791(2)	0.4370(2)	0.067(2)	0.056(1)	0.088(2)	-0.006(1)	-0.014(2)	0.006(1)
C(2)	4*a*	0.1233(6)	0.5297(2)	0.4927(2)	0.059(2)	0.073(2)	0.089(2)	-0.013(1)	-0.006(2)	-0.003(2)
C(3)	4*a*	0.1891(6)	0.5367(2)	0.5703(2)	0.057(2)	0.076(2)	0.088(2)	-0.008(1)	0.004(1)	-0.000(2)
C(4)	4*a*	0.3966(5)	0.5928(2)	0.5946(2)	0.055(2)	0.054(1)	0.080(2)	0.006(1)	-0.005(1)	-0.003(1)
C(5)	4*a*	0.5337(6)	0.6433(2)	0.5365(2)	0.063(2)	0.058(1)	0.096(2)	-0.010(1)	-0.011(2)	0.006(1)
C(6)	4*a*	0.4705(6)	0.6357(2)	0.4596(2)	0.076(2)	0.070(2)	0.089(2)	-0.016(2)	-0.013(2)	0.016(2)
C(7)	4*a*	0.4693(5)	0.5940(2)	0.6759(2)	0.060(2)	0.063(1)	0.083(2)	0.006(1)	0.008(2)	-0.007(1)
C(8)	4*a*	0.6631(6)	0.6431(2)	0.7073(2)	0.072(2)	0.063(1)	0.077(2)	-0.007(1)	0.002(2)	-0.001(1)
C(9)	4*a*	0.7355(5)	0.6331(2)	0.7887(2)	0.062(2)	0.062(1)	0.072(2)	-0.002(1)	0.012(1)	-0.005(1)
C(10)	4*a*	0.9364(5)	0.6998(2)	0.8201(2)	0.059(1)	0.054(1)	0.068(2)	0.002(1)	0.010(1)	-0.005(1)
C(11)	4*a*	1.0393(6)	0.6762(2)	0.8917(2)	0.075(2)	0.071(2)	0.079(2)	-0.007(2)	0.001(2)	0.006(1)
C(12)	4*a*	1.2269(7)	0.7348(3)	0.9230(2)	0.085(2)	0.086(2)	0.090(2)	-0.001(2)	-0.023(2)	-0.001(2)
C(13)	4*a*	1.3178(7)	0.8186(2)	0.8826(2)	0.077(2)	0.075(2)	0.113(3)	-0.011(2)	-0.009(2)	-0.018(2)
C(14)	4*a*	1.2177(7)	0.8438(2)	0.8118(2)	0.100(3)	0.065(2)	0.098(2)	-0.023(2)	0.004(2)	0.002(2)
C(15)	4*a*	1.0271(7)	0.7853(2)	0.7805(2)	0.092(2)	0.059(1)	0.077(2)	-0.008(2)	-0.001(2)	0.002(1)
O(1)	4*a*	0.2120(5)	0.5750(2)	0.3596(1)	0.104(2)	0.102(2)	0.085(2)	-0.038(1)	-0.027(1)	0.023(1)
O(2)	4*a*	0.6410(5)	0.5674(2)	0.8314(1)	0.091(2)	0.097(2)	0.084(1)	-0.034(1)	0.009(1)	0.005(1)

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