

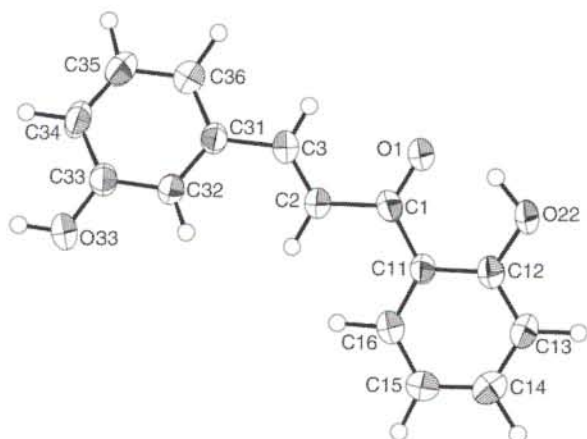
# Crystal structure of *E*-1-(2-hydroxyphenyl)-3-(3-hydroxyphenyl)-2-propen-1-one, C<sub>15</sub>H<sub>12</sub>O<sub>3</sub>

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## Abstract

C<sub>15</sub>H<sub>12</sub>O<sub>3</sub>, monoclinic, *P*12<sub>1</sub>/*c*1 (No. 14), *a* = 8.783(8) Å, *b* = 14.274(9) Å, *c* = 9.316(5) Å, β = 95.39(5)°, *V* = 1162.8 Å<sup>3</sup>, *Z* = 4, *R*<sub>gt</sub>(*F*) = 0.058, *R*<sub>w</sub>(*F*) = 0.058, *T* = 293 K.

## Source of material

Crystals were prepared in a manner similar to that described in [1]; mp 411 K – 412 K.

## Discussion

There is some twisting in the molecule as seen in the values of the C(2)/C(1)/C(11)/C(12) and C(2)/C(3)/C(31)/C(32) torsion angles of –173.0(3)° and 10.2(5)°, respectively. An intramolecular O(1)⋯H–O(22) interaction of 1.61 Å is present. An intermolecular hydrogen bond exists between O(33)–H and O(22)<sup>i</sup> such that H⋯O(22)<sup>i</sup> is 1.82 Å, O(33)⋯O(22)<sup>i</sup> is 2.773(3) Å and O(33)–H(33)⋯O(22)<sup>i</sup> is 178°; symmetry operation *i*: 1+*x*, *y*, 1+*z*.

**Table 3.** Atomic coordinates and displacement parameters (in Å<sup>2</sup>).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>12</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>23</sub>
O(1)	4e	–0.1223(3)	0.3305(2)	–0.2390(2)	0.067(2)	0.046(1)	0.056(2)	–0.004(1)	–0.027(1)	0.007(1)
O(22)	4e	–0.2969(2)	0.2420(2)	–0.4202(2)	0.058(1)	0.053(1)	0.043(1)	–0.003(1)	–0.021(1)	0.007(1)
O(33)	4e	0.4877(3)	0.2164(2)	0.3459(3)	0.068(2)	0.059(2)	0.063(2)	0.000(1)	–0.031(1)	0.007(1)
C(1)	4e	–0.0829(4)	0.2570(2)	–0.1737(3)	0.043(2)	0.044(2)	0.036(2)	0.005(2)	–0.007(2)	0.003(2)
C(2)	4e	0.0386(4)	0.2604(2)	–0.0537(3)	0.045(2)	0.042(2)	0.039(2)	–0.002(2)	–0.009(1)	0.001(2)
C(3)	4e	0.0856(3)	0.3402(2)	0.0072(3)	0.041(2)	0.047(2)	0.041(2)	0.000(2)	–0.007(2)	0.001(2)
C(11)	4e	–0.1558(3)	0.1677(2)	–0.2172(3)	0.038(2)	0.039(2)	0.033(2)	0.002(2)	–0.004(1)	–0.002(1)
C(12)	4e	–0.2600(3)	0.1633(2)	–0.3421(3)	0.041(2)	0.047(2)	0.033(2)	0.002(2)	–0.002(1)	0.001(2)

**Table 1.** Data collection and handling.

Crystal:	yellow, multifaceted, size 0.19 x 0.21 x 0.45 mm
Wavelength:	Mo <i>K</i> <sub>α</sub> radiation (0.7107 Å)
μ:	0.95 cm <sup>–1</sup>
Diffractometer, scan mode:	Rigaku AFC6R, ω/2θ
2θ <sub>max</sub> :	55°
<i>N</i> ( <i>hkl</i> ) <sub>measured</sub> , <i>N</i> ( <i>hkl</i> ) <sub>unique</sub> :	2975, 2803
Criterion for <i>I</i> <sub>obs</sub> , <i>N</i> ( <i>hkl</i> ) <sub>gt</sub> :	<i>I</i> <sub>obs</sub> > 3 σ( <i>I</i> <sub>obs</sub> ), 1357
<i>N</i> ( <i>param</i> ) <sub>refined</sub> :	163
Programs:	TEXSAN [2], R-SAPI88 [3]

**Table 2.** Atomic coordinates and displacement parameters (in Å<sup>2</sup>).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>iso</sub>
H(2)	4e	0.0762	0.1977	–0.0068	0.0808
H(3)	4e	0.0373	0.3992	–0.0240	0.0808
H(13)	4e	–0.4194	0.0777	–0.4787	0.0808
H(14)	4e	–0.3332	–0.0673	–0.3643	0.0808
H(15)	4e	–0.1784	–0.0639	–0.1249	0.0808
H(16)	4e	–0.0573	0.0907	–0.0337	0.0808
H(22)	4e	–0.2528	0.2987	–0.3621	0.0808
H(32)	4e	0.2950	0.2163	0.1338	0.0808
H(33)	4e	0.5638	0.2258	0.4251	0.0808
H(34)	4e	0.4893	0.3881	0.4683	0.0808
H(35)	4e	0.3206	0.5206	0.3579	0.0808
H(36)	4e	0.1783	0.5033	0.1402	0.0808

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Table 3. Continued.

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>12</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>23</sub>
C(13)	4e	-0.3254(4)	0.0797(3)	-0.3894(4)	0.050(2)	0.052(2)	0.048(2)	-0.004(2)	-0.011(2)	-0.008(2)
C(14)	4e	-0.2933(4)	-0.0014(2)	-0.3114(4)	0.063(2)	0.048(2)	0.059(2)	-0.005(2)	-0.004(2)	-0.010(2)
C(15)	4e	-0.1938(4)	0.0012(2)	-0.1857(4)	0.072(3)	0.039(2)	0.063(3)	-0.002(2)	-0.012(2)	0.005(2)
C(16)	4e	-0.1277(4)	0.0845(2)	-0.1400(3)	0.056(2)	0.048(2)	0.044(2)	0.001(2)	-0.013(2)	0.004(2)
C(31)	4e	0.2029(3)	0.3520(2)	0.1297(3)	0.036(2)	0.043(2)	0.036(2)	-0.004(2)	-0.003(1)	0.001(2)
C(32)	4e	0.2958(3)	0.2783(2)	0.1820(3)	0.042(2)	0.042(2)	0.038(2)	-0.005(2)	-0.005(1)	0.001(2)
C(33)	4e	0.4004(4)	0.2918(2)	0.3010(3)	0.043(2)	0.048(2)	0.040(2)	-0.009(2)	-0.008(2)	0.007(2)
C(34)	4e	0.4136(4)	0.3778(3)	0.3691(4)	0.051(2)	0.061(2)	0.042(2)	-0.012(2)	-0.011(2)	-0.006(2)
C(35)	4e	0.3238(4)	0.4507(2)	0.3161(4)	0.061(2)	0.052(2)	0.056(2)	-0.005(2)	-0.009(2)	-0.016(2)
C(36)	4e	0.2159(4)	0.4395(2)	0.1978(4)	0.052(2)	0.046(2)	0.049(2)	-0.003(2)	-0.004(2)	-0.003(2)

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