Crystal structure of *E*-1-(2-hydroxyphenyl)-3-(3-hydroxyphenyl)-2-propen-1-one, $C_{15}H_{12}O_3$

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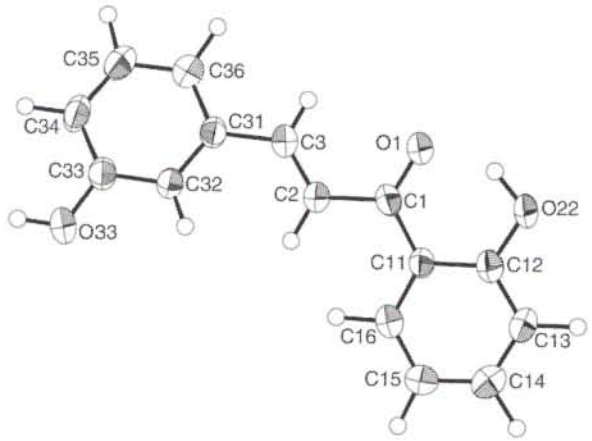

Abstract

$C_{15}H_{12}O_3$, monoclinic, $P12_1/c1$ (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^3, Z = 4, $R_{gt}(F)$ = 0.058, $R_w(F)$ = 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)^i such that H···O(22)^i is 1.82 Å, O(33)···O(22)^i is 2.773(3) Å and O(33)–H(33)···O(22)^i is 178°; symmetry operation i: 1+x, y, 1+z.

Table 1. Data collection and handling.

Crystal:	yellow, multifaceted, size 0.19 x 0.21 x 0.45 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	0.95 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC6R, ω/2θ
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2975, 2803
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 3\ \sigma(I_{obs})$, 1357
$N(param)_{refined}$:	163
Programs:	TEXSAN [2], R-SAPI88 [3]

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

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

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}
O(1)	4*e*	−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)	4*e*	−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)	4*e*	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)	4*e*	−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)	4*e*	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)	4*e*	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)	4*e*	−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)	4*e*	−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)

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Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(13)	4*e*	–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)	4*e*	–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)	4*e*	–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)	4*e*	–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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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)	4*e*	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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