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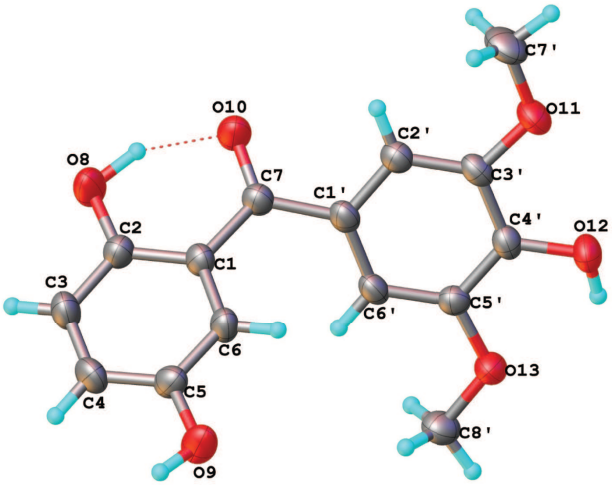
Crystal structure of (2,5-dihydroxyphenyl)-(4-hydroxy-3,5-dimethoxyphenyl)methanone, $C_{15}H_{14}O_6$



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Abstract

$C_{15}H_{14}O_6$, triclinic, $P\bar{1}$ (no. 2), $a = 8.2996(5)$ Å, $b = 8.3739(4)$ Å, $c = 10.7565(5)$ Å, $\alpha = 94.942(3)°$, $\beta = 112.199(4)°$, $\gamma = 102.752(4)°$, $V = 663.09(6)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.044$, $wR_{ref}(F^2) = 0.1134$, $T = 299$ K.

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The crystal structure is shown in the figure, Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The synthesis and the analysis of the title compound are already been reported [1].

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Table 1: Data collection and handling.

Crystal:	Block, size 0.18×0.2×0.3 mm
Wavelength:	Cu K_α radiation (1.54178 Å)
μ:	9.60 cm^{-1}
Diffractometer, scan mode:	Bruker AXS D8-Venture,Triumph-IμS-Cu, φ and ω
$2\theta_{max}$:	118°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	29337, 1900
$N(param)_{refined}$:	201
Programs:	SHELXL [2], OLEX2 [3]

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

Atom	Site	x	y	z	U_{iso}
H(9)	2*i*	0.174(3)	0.987(3)	0.420(3)	0.068
H(12)	2*i*	−0.163(3)	0.106(3)	−0.194(2)	0.051
H(8)	2*i*	0.364(4)	0.337(3)	0.639(3)	0.072
H(7'A)	2*i*	−0.3082	−0.1889	0.1804	0.070
H(7'B)	2*i*	−0.5033	−0.2433	0.0626	0.070
H(7'C)	2*i*	−0.4328	−0.0686	0.1589	0.070
H(2')	2*i*	−0.1221	0.0654	0.2817	0.033
H(6)	2*i*	0.0694	0.5742	0.3115	0.037
H(6')	2*i*	0.2194	0.4249	0.2047	0.031
H(8'A)	2*i*	0.2186	0.5556	0.0252	0.055
H(8'B)	2*i*	0.2502	0.4886	−0.1020	0.055
H(8'C)	2*i*	0.3317	0.4262	0.0357	0.055
H(3)	2*i*	0.5221	0.7632	0.7474	0.046
H(4)	2*i*	0.4128	0.9493	0.6155	0.043

Experimental details

Carbon-bound hydrogen atoms were placed in calculated positions with U_{iso}(H) values of 1.2U_{eq}(C) and 1.5U_{eq}(C) for CH and CH_3 groups. H atoms attached to O atoms were located from Fourier map and were refined isotropically, with O—H distances in the range 0.87(2)–0.90(3) Å.

Discussion

The compound was synthesized from benzoquinone and syringaldehyde, and the structure was determined to confirm its relationship with phenstatin, a potent anti-cancer agent.

Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(11)	2*i*	−0.3294(2)	−0.0800(1)	0.0240(1)	0.0317(7)	0.0286(6)	0.0322(7)	−0.0043(5)	0.0079(5)	−0.0022(5)
O(9)	2*i*	0.1465(2)	0.8841(2)	0.3724(1)	0.079(1)	0.0246(7)	0.0276(7)	0.0227(6)	0.0111(7)	0.0038(5)
O(12)	2*i*	−0.2223(2)	0.0658(1)	−0.1472(1)	0.0326(7)	0.0358(7)	0.0200(6)	−0.0009(5)	0.0028(5)	−0.0038(5)
O(13)	2*i*	0.0699(2)	0.3272(1)	−0.0657(1)	0.0348(7)	0.0321(7)	0.0234(6)	−0.0022(5)	0.0069(5)	0.0040(5)
O(10)	2*i*	0.1989(2)	0.2125(1)	0.4917(1)	0.0617(9)	0.0240(6)	0.0255(7)	0.0109(6)	0.0053(6)	0.0051(5)
O(8)	2*i*	0.4318(2)	0.4493(2)	0.6908(1)	0.0613(9)	0.0323(7)	0.0264(7)	0.0107(6)	−0.0075(6)	0.0058(6)
C(7′)	2*i*	−0.3990(3)	−0.1508(2)	0.1136(2)	0.042(1)	0.038(1)	0.053(1)	−0.0063(8)	0.022(1)	0.0020(9)
C(3′)	2*i*	−0.1803(2)	0.0548(2)	0.0810(2)	0.0231(8)	0.0188(8)	0.0283(9)	0.0038(6)	0.0055(7)	−0.0006(7)
C(2′)	2*i*	−0.0860(2)	0.1168(2)	0.2196(2)	0.0333(9)	0.0220(8)	0.0256(9)	0.0079(7)	0.0112(7)	0.0040(7)
C(1′)	2*i*	0.0631(2)	0.2562(2)	0.2662(2)	0.0310(9)	0.0192(8)	0.0230(9)	0.0084(6)	0.0051(7)	0.0006(6)
C(7)	2*i*	0.1664(2)	0.3160(2)	0.4152(2)	0.0334(9)	0.0228(8)	0.0237(9)	0.0082(7)	0.0071(7)	0.0038(7)
C(1)	2*i*	0.2313(2)	0.4956(2)	0.4742(2)	0.0328(9)	0.0232(8)	0.0194(8)	0.0070(7)	0.0067(7)	0.0012(7)
C(6)	2*i*	0.1608(2)	0.6115(2)	0.3990(2)	0.040(1)	0.0257(9)	0.0186(8)	0.0100(7)	0.0042(7)	−0.0007(7)
C(5)	2*i*	0.2245(2)	0.7791(2)	0.4525(2)	0.047(1)	0.0237(8)	0.0230(9)	0.0124(7)	0.0132(8)	0.0041(7)
C(4′)	2*i*	−0.1243(2)	0.1286(2)	−0.0122(2)	0.0249(8)	0.0212(8)	0.0214(8)	0.0068(6)	0.0032(7)	−0.0021(6)
C(6′)	2*i*	0.1201(2)	0.3315(2)	0.1737(2)	0.0268(8)	0.0174(7)	0.0253(9)	0.0033(6)	0.0032(7)	−0.0001(6)
C(5′)	2*i*	0.0279(2)	0.2661(2)	0.0357(2)	0.0285(8)	0.0199(8)	0.0224(8)	0.0072(6)	0.0072(7)	0.0029(6)
C(8′)	2*i*	0.2307(2)	0.4602(2)	−0.0232(2)	0.0333(9)	0.0338(9)	0.039(1)	0.0022(8)	0.0128(8)	0.0085(8)
C(2)	2*i*	0.3639(2)	0.5546(2)	0.6082(2)	0.036(1)	0.0284(9)	0.0214(9)	0.0071(7)	0.0051(7)	0.0037(7)
C(3)	2*i*	0.4313(3)	0.7243(2)	0.6597(2)	0.041(1)	0.0322(9)	0.0238(9)	0.0046(8)	−0.0006(8)	−0.0045(7)
C(4)	2*i*	0.3641(3)	0.8354(2)	0.5815(2)	0.049(1)	0.0215(8)	0.030(1)	0.0044(7)	0.0116(8)	−0.0039(7)

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