Limin Wang*, Linxiu Zhao and Tingting Qin

Crystal structure of 2-(*tert*-butyl)-6-(hydroxymethyl)-4-methylphenol, C₁₂H₁₈O₂

Table 1: Data collection and handling.

Crystal:	Colourless, block
Size:	0.40 × 0.35 × 0.30 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.08 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, Eos, Gemini, ω -scans
$\theta_{\max}$, completeness:	26°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	15984, 4444, 0.036
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3450
$N(\text{param})_{\text{refined}}$:	265
Programs:	CrysAlis ^{PRO} [1], SHELX [2], OLEX2 [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.08734(6)	0.45506(12)	0.38465(4)	0.0289(3)
H1	0.0934	0.4883	0.4137	0.043*
O2	0.16362(7)	0.54516(11)	0.46794(4)	0.0277(3)
H2	0.1755	0.4818	0.4869	0.042*
O3	0.22389(6)	0.33864(11)	0.52452(4)	0.0273(3)
H3	0.2663	0.3426	0.5127	0.041*
O4	0.36620(7)	0.28735(12)	0.51476(5)	0.0322(3)
H4	0.3618	0.2137	0.5002	0.048*
C1	0.15468(8)	0.40912(15)	0.36579(6)	0.0198(3)
C2	0.15441(9)	0.31608(15)	0.32409(6)	0.0192(3)
C3	0.22364(9)	0.27362(15)	0.30597(6)	0.0207(3)
H3A	0.2250	0.2118	0.2785	0.025*
C4	0.29107(9)	0.31850(16)	0.32662(6)	0.0227(4)
C5	0.28857(9)	0.41045(15)	0.36756(6)	0.0220(4)
H5	0.3329	0.4414	0.3821	0.026*
C6	0.22116(9)	0.45741(15)	0.38728(6)	0.0201(3)
C7	0.22060(10)	0.56577(16)	0.42887(6)	0.0273(4)
H7A	0.2689	0.5677	0.4459	0.033*
H7B	0.2129	0.6533	0.4124	0.033*
C8	0.36410(9)	0.26631(19)	0.30537(7)	0.0353(4)
H8A	0.4036	0.3260	0.3158	0.053*
H8B	0.3617	0.2628	0.2679	0.053*
H8C	0.3734	0.1770	0.3189	0.053*
C9	0.08113(9)	0.26602(16)	0.29950(6)	0.0252(4)
C10	0.03578(10)	0.38732(18)	0.27933(7)	0.0364(5)
H10A	0.0240	0.4465	0.3079	0.055*
H10B	−0.0095	0.3553	0.2636	0.055*
H10C	0.0644	0.4360	0.2538	0.055*
C11	0.09518(10)	0.17168(18)	0.25300(7)	0.0339(4)
H11A	0.1237	0.2188	0.2270	0.051*
H11B	0.0484	0.1439	0.2383	0.051*
H11C	0.1223	0.0932	0.2645	0.051*
C12	0.03578(10)	0.18677(19)	0.34031(7)	0.0342(4)

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Abstract

C₁₂H₁₈O₂, orthorhombic, *Pbca* (no. 61), $a = 17.9560(6)$ Å, $b = 9.8553(3)$ Å, $c = 25.5955(7)$ Å, $V = 4529.4(2)$ Å³, $Z = 16$, $R_{\text{gt}}(F) = 0.0490$, $wR_{\text{ref}}(F^2) = 0.1162$, $T = 107(10)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Equimolar amounts of 2,6-di-*tert*-butylphenol (98%, Aladdin) and paraformaldehyde (>99%, Aladdin) were mixed and stirred at 373 K for 10 h in the presence of base. The solution was cooled to room temperature, which was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20/1) to afford the product as a white solid. The crude product was recrystallized from hexane.

***Corresponding author: Limin Wang**, School of Chemical Engineering and Technology, North University of China, Taiyuan, Shanxi Province, P.R. China, e-mail: wanglimin@nuc.edu.cn
Linxiu Zhao and Tingting Qin: School of Chemical Engineering and Technology, North University of China, Taiyuan, Shanxi Province, P.R. China

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H12A	0.0638	0.1093	0.3517	0.051*
H12B	−0.0102	0.1572	0.3250	0.051*
H12C	0.0255	0.2444	0.3697	0.051*
C13	0.22202(9)	0.24753(15)	0.56586(6)	0.0201(3)
C14	0.15357(9)	0.19605(15)	0.58331(6)	0.0212(3)
C15	0.15659(9)	0.10781(16)	0.62599(6)	0.0234(4)
H15	0.1120	0.0744	0.6392	0.028*
C16	0.22232(10)	0.06710(16)	0.64980(6)	0.0264(4)
C17	0.28867(10)	0.11780(17)	0.63021(6)	0.0279(4)
H17	0.3335	0.0902	0.6450	0.033*
C18	0.28943(9)	0.20929(16)	0.58879(6)	0.0238(4)
C19	0.36239(10)	0.26875(18)	0.57046(7)	0.0326(4)
H19A	0.3698	0.3558	0.5874	0.039*
H19B	0.4026	0.2093	0.5812	0.039*
C20	0.22143(11)	−0.03259(19)	0.69471(7)	0.0390(5)
H20A	0.2377	0.0121	0.7260	0.059*
H20B	0.2543	−0.1068	0.6870	0.059*
H20C	0.1718	−0.0664	0.6996	0.059*
C21	0.07889(9)	0.23146(17)	0.55694(6)	0.0260(4)
C22	0.06248(10)	0.38388(18)	0.56384(7)	0.0351(4)
H22A	0.1049	0.4357	0.5528	0.053*
H22B	0.0522	0.4025	0.5999	0.053*
H22C	0.0201	0.4084	0.5430	0.053*
C23	0.08113(10)	0.19249(19)	0.49872(6)	0.0325(4)
H23A	0.0911	0.0971	0.4955	0.049*
H23B	0.1197	0.2430	0.4815	0.049*
H23C	0.0340	0.2131	0.4829	0.049*
C24	0.01359(10)	0.1535(2)	0.58122(8)	0.0397(5)
H24A	0.0098	0.1756	0.6176	0.060*
H24B	0.0218	0.0577	0.5774	0.060*
H24C	−0.0318	0.1782	0.5638	0.060*

Experimental details

All the Friedel pairs were merged [3]. All H atoms were positioned geometrically and treated as riding, with C—H bond

lengths constrained to 0.9 Å for phenyl ring H and 0.9 Å for methyl H atoms, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for phenyl ring H atom and $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and ethyl H atoms.

Discussion

Hindered phenols had been widely used in high polymer compound as antioxidant [4].

There are two crystallographically independent molecules in the asymmetric unit (cf. the figure). Geometric parameters are in the expected ranges.

In the crystal structure, the crystal packing is stabilized in layers and held together by van der Waals interactions and classical intermolecular O—H···O hydrogen bonds and intramolecular O—H···O hydrogen bonds.

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