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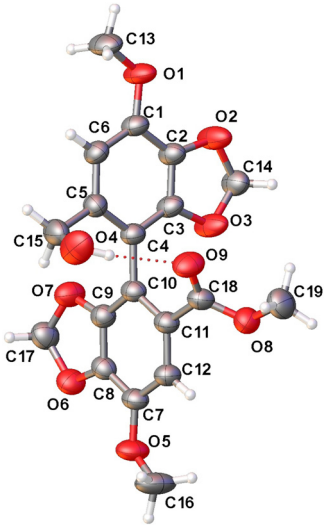
The crystal structure of bicyclol, $C_{19}H_{18}O_9$



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Abstract

$C_{19}H_{18}O_9$, monoclinic, $P2_1/c$ (no. 14), a = 8.82839(18) Å, b = 15.3431(3) Å, c = 13.4413(3) Å, β = 97.3429(18)°, V = 1805.76(6) Å^3, Z = 4, $R_{gt}(F)$ = 0.0399, $wR_{ref}(F^2)$ = 0.1167, T = 297 K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of materials

The title compound (bicyclol, systematic name: methyl 5′-(hydroxymethyl)-7,7′-dimethoxy-[4,4′-bibenzo[*d*][1,3]dioxole]-5-carboxylate) was bought from Shanghai Aladdin Biochemical Technology Co., Ltd. About 50 mg bicyclol powder was placed into a 10 ml penicillin bottle, followed by addition of 8 ml methanol. The mixture was shaken intermittently to ensure complete dissolution. The penicillin bottle was left open and placed in a fume hood. After 3 days, block-shaped crystals precipitated.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.25 × 0.20 × 0.18 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	0.99 mm^{-1}
Diffractometer, scan mode:	Rigaku synergy, ω scans
θ_{max}, completeness:	76.2°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	17413, 3638, 0.031
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3,151
$N(param)_{refined}$:	260
Programs:	Rigaku,[1] Olex2,[2] SHELX[3,4]

2 Experimental details

The positions of hydrogen atoms on carbon atoms were calculated geometrically and refined using the riding model. Their coordinates and displacement parameters were constrained to ride on the carrier atom. The hydrogen atom on the oxygen atom was located from difference Fourier map inspection and refined with U_{iso}(H) = 1.5U_{eq}(O). The distance between the hydrogen atom and the oxygen atom was refined freely. A DFIX restrain was used to get a better model for the hydrogen atom.

3 Comment

Bicyclol is a synthetic drug for the treatment of chronic viral hepatitis. Its structure is similar to that of bifendate,[5] with only one substituent difference. It exhibits significant hepatoprotective effects and certain antiviral activity against hepatitis viruses.[6] Bicyclol is safe for the treatment of chronic hepatitis B and chronic hepatitis C, and it is effective in improving liver function.[7]

The titled compound was crystallized in $P2_1/c$ space group with one molecule in its asymmetric unit. The bond lengths and angles within all moieties are in the expected

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ranges. The torsion angle between C3, C4, C10 and C11 is 75.8(2)°, indicating that the two benzene rings in the structure are nearly perpendicular. The torsion angle between C17, O7, C9 and C8 is 5.99(17)°, and the torsion angle between C14, O2, C2 and C3 is 7.3(2)°, suggesting that the two dioxolane rings in the structure are essentially planar. Additionally, there is an intramolecular hydrogen bond between the O4 and O9 atoms in the structure, with a distance of 2.984(2) Å between them.

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Conflict of interest: The authors declare no conflicts of interest regarding this article.

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