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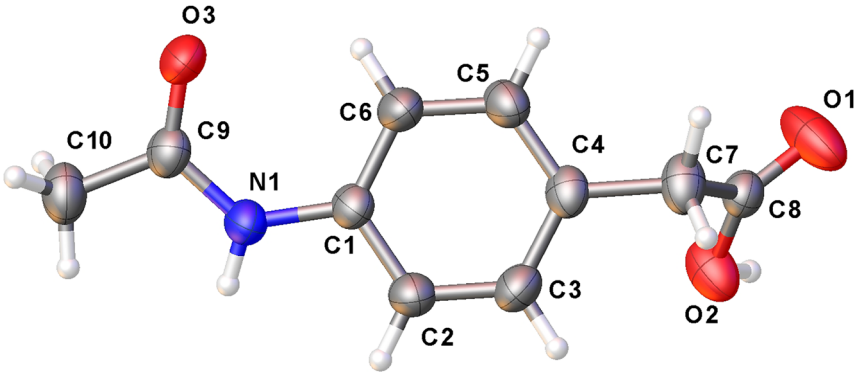
The crystal structure of actarit, $C_{10}H_{11}NO_3$



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Abstract

$C_{10}H_{11}NO_3$, orthorhombic, *Pbca* (no. 61), a = 13.3367(3) Å, b = 7.8091(2) Å, c = 18.7826(3) Å, V = 1956.16(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0393, $wR_{ref}(F^2)$ = 0.1131, T = 297 K.

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

Table 1: Data collection and handling.

Crystal:	Colourless plate
Size:	0.25 × 0.25 × 0.10 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	0.81 mm^{-1}
Diffractometer, scan mode:	Rigaku Synergy, ω scans
θ_{max}, completeness:	75.8°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9658, 1963, 0.033
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1,734
$N(param)_{refined}$:	135
Programs:	Rigaku,[1] Olex2,[2] SHELX[3,4]

1 Source of materials

The title compound (actarit, systematic name: methyl 5′-(hydroxymethyl)-7,7′-dimethoxy-[4,4′-bibenzo[*d*][1,3]dioxole]-5-carboxylate) was bought from Shanghai Bide Pharmatech Co., Ltd. About 20 mg actarit powder was placed into a 10 ml penicillin bottle, followed by addition of 3 ml methanol. The mixture was shaken intermittently to ensure complete dissolution. The penicillin bottle was left open and placed in a fume hood. After 2 days, plate-shaped crystals precipitated. System name: 4-acetylaminophenylacetic acid.

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 oxygen atom and nitrogen atom were located from difference Fourier map inspection and refined with U_{iso}(H) = 1.5U_{eq}(O) or U_{iso}(H) = 1.5U_{eq}(N). The distance between the hydrogen atom and the oxygen atom or the nitrogen atom were refined freely. A DFIX restrain was used to get a better model for the hydrogen atom.

3 Comment

Actarit is an immunomodulatory agent primarily used in the treatment of rheumatoid arthritis (RA).[5] It functions by

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modulating the immune system to reduce inflammation and joint damage.[6] The exact mechanism of action of actarit is not fully understood, but research suggests that it may work by inhibiting the production of certain inflammatory mediators or by modulating T-cell function.[7,8]

The titled compound was crystallized in *Pbca* space group with one molecule in its asymmetric unit. The bond lengths and angles within this simple molecule are in the expected ranges. The bond length between O1 and C8 is 1.1954(17) Å, and the bond length between O2 and C8 is 1.2997(16) Å, indicating that the terminal group is an un-ionized carboxyl group. The torsion angle of C1–N1–C9–O3 is −4.2(2)°, suggesting that the amide group and the benzene ring are not completely coplanar. This structure extends into a complex three-dimensional network through hydrogen bonding.

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

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