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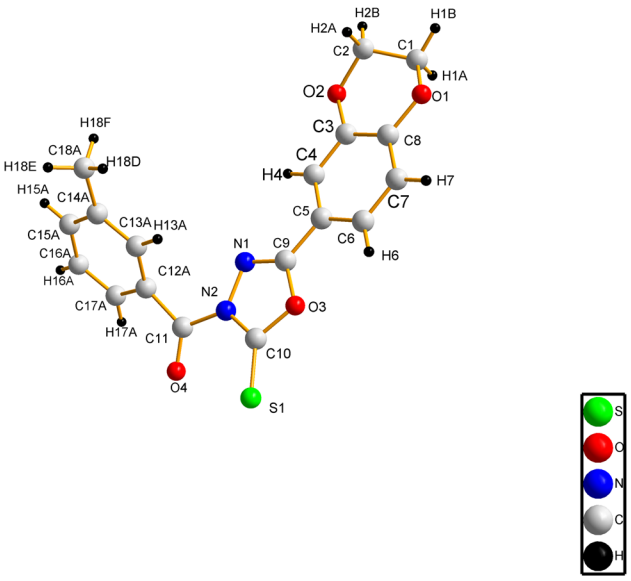
The crystal structure of (5-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-sulfanylidene-1,3,4-oxadiazol-3(2*H*)-yl)(3-methylphenyl)methanone, $C_{18}H_{14}N_2O_4S$



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Abstract

$C_{18}H_{14}N_2O_4S$, triclinic, $P\bar{1}$ (no. 2), a = 8.0785(6) Å, b = 8.4022(6) Å, c = 13.7881(10) Å, α = 81.537(2)°, β = 75.581(2)°, γ = 64.198(2)°, V = 815.24(10) Å^3, Z = 2, $R_{gt}(F)$ = 0.0437, $wR_{ref}(F^2)$ = 0.1159, T = 273 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.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.47 × 0.35 × 0.32 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.23 mm^{-1}
Diffractometer, scan mode:	Bruker APEX2, φ and ω scans
θ_{max}, completeness:	27.5°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8461, 3683, 0.021
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2,784
$N(param)_{refined}$:	292
Programs:	Bruker[1], Olex2[2], SHELX[3,4]

1 Source of materials

5-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-1,3,4-oxadiazole-2-thiol (0.236 g, 1 mmol), potassium carbonate (0.207, 1.5 mmol) and 3-methylbenzoylchloride (0.155 g, 1 mmol) were mixed in dry *N*,*N*-dimethylformamide (20 mL) and stirred for 4 h. The precipitate was collected by filtration, washed with cold ethanol, dried, and recrystallized from petroleum ether/ethyl acetate. Colourless block crystals were obtained by slow evaporation.

2 Experimental details

Absorption corrections were applied by using multi-scan program.[1] Using Olex2,[2] the structure was solved with the ShelXT[3] structure solution program and refined with the ShelXL[4] refinement package.

3 Comment

Several groups have long been intrigued by 1,3,4-oxadiazole-2(3*H*)-thione derivatives containing a 1,4-benzodioxane skeleton, because of their diverse biological activities, including anti-tumor, antibacterial, anti-inflammatory, and adrenergic antagonism.[5,6]

The molecular structure comprises four distinct planes: the benzene ring plane, the oxadiazole ring plane, the

benzene ring plane within the 1,4-benzodioxane structure, and the dioxane ring plane. These planes collectively form the fundamental framework of the molecule. The dihedral angles between the benzene ring plane and the other three planes are 52.14°, 51.18°, and 50.7°, respectively. The dihedral angles between the oxadiazole plane and the remaining two planes are 5.66° and 4.06°. Additionally, the dihedral angle between the benzene ring plane and the dioxane ring plane within the 1,4-benzodioxane structure is 1.81°. The single-crystal structure analysis confirms that all bond lengths and bond angles of the compound fall within a reasonable range.[7]

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