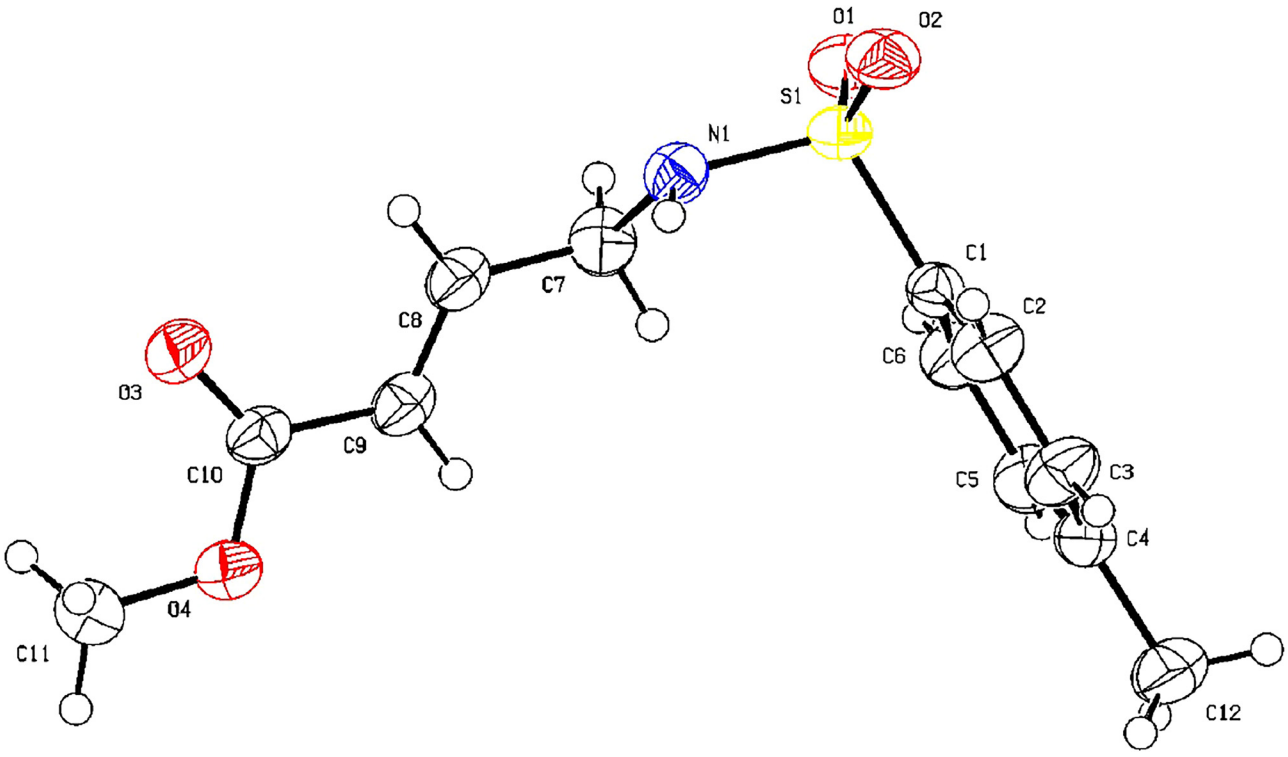
Shanshan Weng*

Crystal structure of methyl (*E*)-4-((4-methylphenyl) sulfonamido)but-2-enoate, $C_{12}H_{15}NO_4S$



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Abstract

$C_{12}H_{15}NO_4S$, monoclinic, $P2_1/c$ (no. 14), a = 16.4941(3) Å, b = 6.95290(10) Å, c = 11.8288(2) Å, β = 106.986(2)°, V = 1297.37(4) Å^3, Z = 4, $R_{gt}(F)$ = 0.0440, $wR_{ref}(F^2)$ = 0.1226, T = 220(1) 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.

***Corresponding author: Shanshan Weng**, Department of Hematology, The Dingli Clinical College of Wenzhou Medical University (The Second Affiliated Hospital of Shanghai University, Wenzhou Central Hospital), Zhejiang, 325000, China, E-mail: wengshanshan@wmu.edu.cn. https://orcid.org/0000-0003-1718-2747

1 Source of materials

To the mixture of 4-methylbenzenesulfonamide (0.3 mmol) and K_2CO_3 (0.3 mmol), the methyl (*E*)-4-bromobut-2-enoate (0.3 mmol) was successively added into the tube. The reaction mixture was stirred at room temperature under air for 3 h. The resulting mixture was quenched with saturated NH_4Cl solution (10 mL), and the mixture was extracted with AcOEt (3 × 25 mL). The organic layers were dried over $MgSO_4$ and concentrated at

Table 1: Data collection and handling.

Crystal:	Clear pale colourless block
Size:	0.13 × 0.12 × 0.10 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	2.30 mm^{-1}
Diffractometer, scan mode:	Oxford Diffraction, ω scans
θ_{max}, completeness:	71.8°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5222, 2489, 0.015
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2,401
$N(param)_{refined}$:	170
Programs:	Oxford,[1] Olex2,[2] SHELX[3,4]

reduced pressure. The residue was purified by column chromatography on silica gel providing the title compound. The colorless crystals of the title compound were obtained by slow evaporation of a CH_3Cl solution at room temperature.

2 Experimental details

Position of the H atoms were calculated based on geometric criteria (C–H = 0.97 and 0.93 for methyl and aromatic atoms, respectively) than have been placed in their calculated position and refined isotropically using a riding model with U_{iso}(H) = 1.5 U_{eq} for methyl and U_{iso}(H) = 1.2 for all others.

3 Comment

Methyl crotonate is a valuable *α*,*β*-unsaturated ester widely utilized in organic synthesis and industrial applications.[4,5] Its conjugated double bond and ester functionality make it a versatile intermediate for polymerization, catalysis, and fine chemical production. Sulfonamide represents privileged structural motif that plays a pivotal role in modern drug discovery and development, prominently featured in natural product architectures, therapeutic agents, and bioactive compounds.[6–10] The integration of methyl crotonate and sulfonamide moieties in hybrid compounds is anticipated to demonstrate significant biological activity, attributed to the complementary interactions of their functional groups.

The solid structure of the title complex is depicted in the figure. One carbon-oxygen double bond exists in the compound, the C–O double bond distance (C10–O3) is 1.207(2) Å. The angle of C10–O4–C11 is 116.04(14)°. The bond distances of S–O are 1.4293(13) Å (S1–O1) and 1.4324(12) Å (S1–O2). The other bond distances and angles are in their normal ranges according to the previously reported compounds.[11]

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