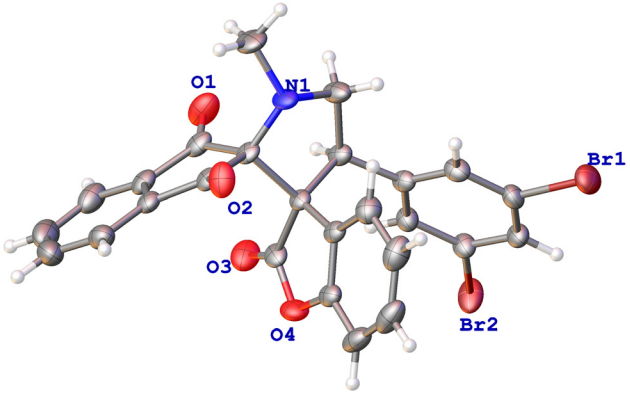
Yi-Hui Chai, Zhi-Ling Fan, Zhang-Chao Dong, Yang Shi, Li-Juan Liu, Bo-Wen Pan* and Fang-Fang Yang*

Synthesis and crystal structure (3R,4′S)-4′-(3,5-dibromophenyl)-1′-methyl-2*H*-dispiro [benzofuran-3,3′-pyrrolidine-2′,2″-indene]-1″,2,3″-trione, $C_{26}H_{17}Br_2NO_4$



https://doi.org/10.1515/ncrs-2025-0299
Received July 1, 2025; accepted August 21, 2025;
published online October 23, 2025

Abstract

$C_{26}H_{17}Br_2NO_4$, triclinic, $P\bar{1}$ (no. 2), a = 8.3900(2) Å, b = 11.9445(2) Å, c = 12.4155(2) Å, α = 74.4620(10)°, β = 81.802(2)°, γ = 70.601(2)°, V = 1128.72(4) Å^3, Z = 2, $R_{gt}(F)$ = 0.0449, $wR_{ref}(F^2)$ = 0.1228, T = 249(1) K.

CCDC no.: 2481627

The molecular structure is shown in the figure. Table 1 contains the crystallographic data and 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:	Clear pale yellow block
Size:	0.14 × 0.12 × 0.10 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	4.84 mm^{-1}
Diffractometer, scan mode:	Rigaku XtaLAB, ω scans
θ_{max}, completeness:	71.7°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9075, 4256, 0.022
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4,156
$N(param)_{refined}$:	300
Programs:	Rigaku,[1] Olex2,[2] Shelx[3]

1 Source of material

The 3-(3,5-dibromobenzyl)benzofuran-2(3*H*)-one (2 mmol, 0.86 g) was dissolved in THF (2 mL). Then Ninhydrin hydrate acid (0.0713 g, 0.4 mmol) and Sarcosine (0.0535 g, 0.6 mmol) were added and stirred at 40 °C for 8 h. Then, the crude product was subjected to flash column chromatography on silica gel (PE/EA = 3:1) to afford the product.

2 Comment

Benzofuranone is an important bioactive compound. They have great potential for application in the field of organic synthesis, It is an intermediate used in many compounds, with anti-tumor, antibacterial, and neuroprotective effects.[4–6] Therefore, the synthesis of benzofuranone has always been a hot topic in the medical field. The basic structure of the title compound is constructed by two benzofurans connected together. There are two bromine atoms on the benzene ring and one ketone carbonyl on each of the two pentagonal rings. The bond lengths and angles of the title compound are in the normal range and consistent with previously reported structures.[7–9]

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Acknowledgements: This research was Guizhou Provincial Science and Technology Support Program Project (Qiankehe

Support [2025] General 110), Guizhou Provincial Basic Research Program (Natural Science) (No. ZK [2023] general 404 and ZK [2024] general 370), the Guiyang City Science and Technology Plan Project (NO. [2024]2–37), the Research Project on Traditional Chinese Medicine and Ethnic Medicine Science and Technology of Guizhou Provincial Administration of Traditional Chinese Medicine (QZYY-2024–130).

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