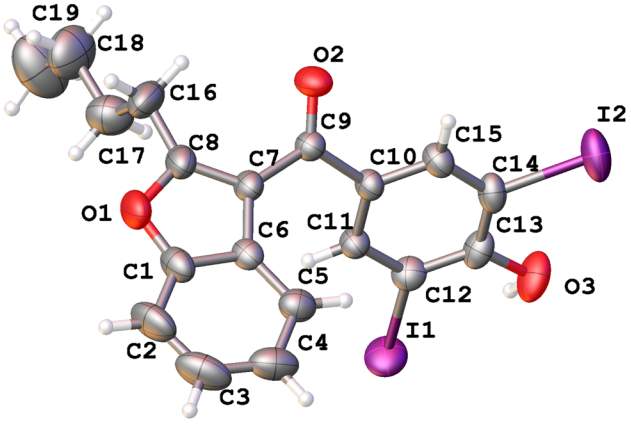
Fengfeng Wang, Caiyu Zhang, Xiaowen Hu, Lin Luan and Yang Liu*

# The crystal structure of (2-butyl-benzofuran-3-yl)(4-hydroxy-3,5-diiodophenyl)methanone, $C_{19}H_{16}I_2O_3$

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**Abstract**

$C_{19}H_{16}I_2O_3$, triclinic, $P\bar{1}$ (no. 2), $a$ = 8.9049(1) Å, $b$ = 9.1514(1) Å, $c$ = 12.0282(2) Å, $\alpha$ = 101.511(1)°, $\beta$ = 101.691(1)°, $\gamma$ = 93.386(1)°, $V$ = 935.49(2) Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0454, $wR_{ref}(F^2)$ = 0.1289, 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.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Prism, colourless |
| Size: | 0.5 × 0.2 × 0.1 mm |
| Wavelength: | Cu $K\alpha$ radiation (1.54184 Å) |
| $\mu$: | 26.52 mm$^{-1}$ |
| Diffractometer, scan mode: | XtaLAB Synergy R, $\omega$-scans |
| $\theta_{max}$, completeness: | 76.4°, > 99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 17784, 3781, 0.046 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs}$ > 2 $\sigma(I_{obs})$, 3,483 |
| $N(param)_{refined}$: | 222 |
| Programs: | CrysAlis$^{PRO}$,[1] Olex2,[2] Shelx[3,4] |

## 1 Source of materials

The title compound was bought from Guangzhou Dmstandards Co., Ltd. About 50 mg powder was placed into a 10 ml penicillin bottle, followed by addition of 5 ml ethanol. After all the powder was dissolved, the penicillin bottle was left open and placed in a fume hood. After 5 days, prism-shaped crystals were harvested.

## 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 was located from difference Fourier map inspection and refined with $U_{iso}$(H) = 1.5$U_{eq}$(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

Amiodarone has become an important drug for the treatment of supraventricular and ventricular arrhythmias, in short-term inpatient and outpatient settings.[5] The title compound is an impurity of the synthesis of amiodarone,[6] and this compound is usually controlled as a process impurity.[7] A certain inhibition effect of thyroxine deiodination is observed in this compound.[8]

***Corresponding author: Yang Liu**, Institute for Chemical Drug Control National, Institutes for Food and Drug Control, Beijing, 102629, P.R. China, E-mail: yangliu@nifdc.org.cn
**Fengfeng Wang, Caiyu Zhang, Xiaowen Hu and Lin Luan**, Institute for Chemical Drug Control, National Institutes for Food and Drug Control, Beijing, 102629, P.R. China. https://orcid.org/0009-0002-3830-9831 (F. Wang). https://orcid.org/0000-0002-9416-8650 (C. Zhang). https://orcid.org/0000-0003-0835-2476 (X. Hu)

The titled compound was crystallized in $P\bar{1}$ space group with one molecule in its asymmetric unit. The bond lengths and angles within these moieties are in the expected ranges.[9] The four atoms, including C7 and C10 attached to the carbonyl group, are coplanar. However, the benzofuran ring and benzene ring connected to the carbonyl group are not in the same plane. The dihedral angle between the benzofuran ring and the benzene ring can be represented by the torsion angle C6–C7–C9–C10, with a value of 39.4(6)°. The butyl group attached to the benzofuran ring adopts a typical *all-trans* conformation. The only hydroxyl group in the molecule forms an O2–H2···O3$^{1-x,1-y,1-z}$ hydrogen bond with the carbonyl group of an adjacent molecule, and the donor acceptor length of this hydrogen bond is 3.027(6) Å. In addition to hydrogen bonding, $\pi$–$\pi$ stacking interactions also could be observed, with centroid-centroid distance of 3.58 Å, and shift distance of 0.63 Å.

**Author contribution:** All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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

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