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Crystal structure of 3-allyl-4-(2-bromoethyl)-5-(4-methoxyphenyl)-2-phenylfuran, $C_{22}H_{21}BrO_2$

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Abstract

$C_{22}H_{21}BrO_2$, monoclinic, $P2_1/c$ (no. 14), $a = 22.175(2)$ Å, $b = 5.8375(6)$ Å, $c = 14.8729(14)$ Å, $\beta = 100.936(1)^\circ$, $V = 1890.3(3)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0343$, $wR_{ref}(F^2) = 0.0839$, $T = 296(2)$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	$0.20 \times 0.18 \times 0.16$ mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	2.19 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	26.4° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	13,804, 3862, 0.026
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2606
$N(\text{param})_{\text{refined}}$:	246
Programs:	Bruker [1], SHELX [2]

Source of material

The title compound was synthesized according to our previous reported method, only the (4-methoxyphenyl) (1-(*p*-tolylethynyl) cyclopropyl)methanone was replaced by (4-methoxyphenyl) (1-(phenylethynyl)cyclopropyl)methanone [3]. The crystal suitable for single crystal structure determination was obtained by recrystallization from tetrahydrofuran at room temperature.

Experimental details

All H atoms were included in calculated positions and refined as riding atoms with C–H = 0.93–0.97 Å, with $U_{\text{iso}} = 1.5 U_{\text{eq}}(\text{C})$ for methyl H

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} [*] /U _{eq}
Br1	0.19913 (2)	0.11721 (5)	0.58231 (2)	0.07259 (13)
O1	0.25684 (8)	0.8688 (3)	0.29775 (13)	0.0648 (5)
O2	−0.01240 (10)	0.6470 (4)	0.09392 (14)	0.0846 (6)
C1	0.21593 (11)	0.7301 (4)	0.33181 (19)	0.0576 (7)
C2	0.24030 (12)	0.6690 (4)	0.4188 (2)	0.0583 (7)
C3	0.29994 (12)	0.7735 (4)	0.4413 (2)	0.0642 (7)
C4	0.30784 (12)	0.8922 (4)	0.3659 (2)	0.0670 (7)
C5	0.15738 (12)	0.6980 (4)	0.27012 (18)	0.0560 (6)
C6	0.11978 (12)	0.5091 (5)	0.27505 (19)	0.0647 (7)
H6	0.133117	0.395143	0.317935	0.078*
C7	0.06316 (13)	0.4864 (5)	0.21787 (19)	0.0676 (7)
H7	0.038800	0.359235	0.223124	0.081*
C8	0.04278 (13)	0.6513 (5)	0.15330 (19)	0.0655 (7)
C9	0.08002 (14)	0.8386 (5)	0.1461 (2)	0.0708 (8)
H9	0.066937	0.950232	0.102090	0.085*
C10	0.13588 (13)	0.8607 (4)	0.20323 (19)	0.0655 (7)
H10	0.160118	0.987725	0.197201	0.079*
C11	−0.05025 (14)	0.4501 (6)	0.0955 (2)	0.0943 (10)
H11A	−0.027821	0.315260	0.084901	0.142*
H11B	−0.086290	0.463583	0.048487	0.142*
H11C	−0.062121	0.438954	0.154141	0.142*
C12	0.35502 (13)	1.0473 (5)	0.3453 (2)	0.0705 (8)
C13	0.41696 (13)	1.0052 (5)	0.3779 (3)	0.0924 (10)
H13	0.428885	0.873088	0.411497	0.111*
C14	0.46111 (16)	1.1584 (7)	0.3608 (3)	0.1053 (12)
H14	0.502426	1.129507	0.383561	0.126*
C15	0.44432 (18)	1.3508 (7)	0.3108 (3)	0.1068 (12)
H15	0.474182	1.452939	0.299420	0.128*
C16	0.38348 (18)	1.3948 (6)	0.2770 (3)	0.0995 (11)
H16	0.372265	1.526487	0.242665	0.119*
C17	0.33849 (14)	1.2433 (5)	0.2937 (2)	0.0797 (8)
H17	0.297312	1.273365	0.270412	0.096*
C18	0.21078 (11)	0.5314 (4)	0.48488 (18)	0.0589 (6)
H18A	0.221628	0.597685	0.545610	0.071*
H18B	0.166466	0.538227	0.466192	0.071*
C19	0.23132 (12)	0.2853 (4)	0.4880 (2)	0.0658 (7)
H19A	0.275841	0.278759	0.500898	0.079*
H19B	0.216926	0.214340	0.428813	0.079*
C20	0.34128 (14)	0.7729 (5)	0.5333 (3)	0.0919 (10)
H20A ^a	0.317788	0.756748	0.581689	0.110*
H20B ^a	0.365073	0.913174	0.543041	0.110*
H20C ^b	0.314614	0.815673	0.575217	0.110*
H20D ^b	0.368077	0.903453	0.531420	0.110*
C21 ^a	0.3836 (3)	0.5629 (12)	0.5304 (5)	0.075 (3)
H21A ^a	0.398778	0.533492	0.477423	0.090*
C22 ^a	0.3982 (4)	0.4288 (15)	0.5994 (6)	0.112 (3)
H22A ^a	0.383296	0.456453	0.652781	0.134*
H22B ^a	0.423678	0.303759	0.596059	0.134*
C21B ^b	0.3832 (4)	0.5905 (12)	0.5848 (6)	0.072 (3)
H21B ^b	0.394940	0.588107	0.648282	0.087*
C22B ^b	0.4008 (4)	0.4407 (16)	0.5325 (7)	0.081 (3)
H22C ^b	0.387837	0.450450	0.469410	0.097*
H22E ^b	0.426607	0.322024	0.557629	0.097*

^aOccupancy: 0.539(11), ^bOccupancy: 0.461(11).

atoms and 1.2 U_{eq}(C) for the remaining H atoms. Some atoms are disordered over two positions. The two parts overlapped each other with site occupation factors of 0.539 and 0.461. The disorder is omitted in the figure for clarity.

Comment

Furan derivatives have attracted more and more attention due to their wide variety of biological and pharmacological activities [3–12]. Recently we have reported the structure of the structurally related 3-allyl-4-(2-bromoethyl)-5-(4-methoxyphenyl)-2-(*p*-tolyl)furan [3]. In continuation of our research on furan derivatives, the molecular and crystal structure of the title compound were determined.

In the crystal structure, the asymmetric unit of the title compound consists of one formula unit (*cf.* Figure). The bond lengths are comparable with those found in our previous work [3] and that of others [12, 13]. The dihedral angle formed by the two aromatic rings is 22.319(1) Å. The furan ring and the two aromatic rings form dihedral angles of 26.389(1)° and 37.263(1)°, respectively. In the crystal, weak intermolecular C–H⋯Br hydrogen bonds link the molecules into one dimensional chains along the *b* axis.

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