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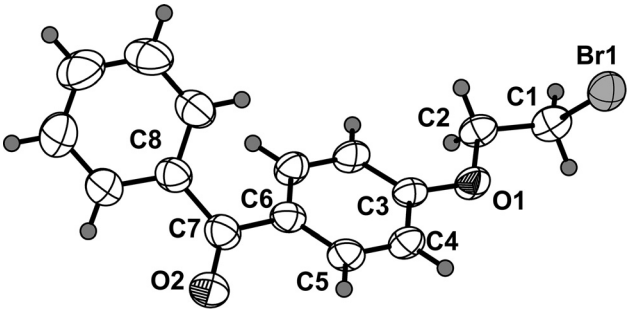
The crystal structure of (4-(2-bromoethoxy)-phenyl)(phenyl)methanone, $C_{15}H_{13}BrO_2$



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Abstract

$C_{15}H_{13}BrO_2$, monoclinic, $P2_1/c$ (no. 14), a = 5.6574(9) Å, b = 9.7821(16) Å, c = 24.251(4) Å, β = 93.265(4)°, V = 1339.9(4) Å^3, Z = 4, $R_{gt}(F)$ = 0.0428, $wR_{ref}(F^2)$ = 0.0930, T = 273 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:	Colourless block
Size:	0.19 × 0.17 × 0.15 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	3.06 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	28.5°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9101, 3338, 0.036
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2414
$N(param)_{refined}$:	163
Programs:	CrysAlis^{PRO} [1], Shelx [2, 3]

Source of material

4-Hydroxybenzophenone (1.98 g, 10 mmol), 1,2-dibromoethane (9.4 g, 50 mmol) and K_2CO_3 (4.1 g, 30 mmol) were added to 60 mL of acetone at room temperature. The mixture was refluxed for 48 h and then cooled to room temperature. The reaction solution was filtered and the filtrate evaporated under reduced pressure to get an yellow oil. The product was purified by silica gel column chromatography (dichloromethane as the eluent) to obtain a white solid, which is recrystallized from methanol to obtain a white block crystal.

Experimental details

The data were scaled and corrected for absorption using SADABS-2016/2 [2, 3]. The hydrogen atoms were placed at calculated positions as riding atoms.

Comment

With the advantages of simple synthesis and low price, benzophenone derivatives were widely used in the areas of photoinitiator [4], sunscreen [5–7], photoluminescent materials [8, 9], organic field-effect transistor [10], pesticide [11] and so on. In the field of hydrogen scavenging photoinitiator, different fuctional groups (such as acryloyl, acylamino, propargyl ect.) can be introduced into the backbone of benzophenone to improve photoinitiating activities [12–14]. So design, synthesis and photoinitiation activity study of novel benzophenone derivatives obviously become an important subject. Due to the bromine atom at the end of the skeleton in the title molecular structure, water-soluble photoinitiators with novel structures can be prepared using (4-(2- bromoethoxy)phenyl)(phenyl)methanone as reactant in a nucleophilic reaction (introducing polysiloxane or quaternary ammonium ions) [15].

In the structure of the title molecule, the bond length of C1–Br1 is 1.937(3) Å. The bond lengths of C2–O1, C7–O2 and

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Br1	−0.04588 (5)	0.87602 (3)	0.43624 (2)	0.05795 (13)
O1	0.2492 (3)	0.60096 (17)	0.45573 (8)	0.0494 (5)
O2	0.4810 (4)	0.0087 (2)	0.37092 (10)	0.0732 (6)
C1	0.2513 (5)	0.8380 (3)	0.47695 (12)	0.0510 (7)
H1A	0.3485	0.9198	0.4780	0.061*
H1B	0.2204	0.8141	0.5147	0.061*
C2	0.3833 (5)	0.7244 (3)	0.45167 (11)	0.0468 (6)
H2A	0.4068	0.7448	0.4132	0.056*
H2B	0.5374	0.7137	0.4708	0.056*
C3	0.3308 (4)	0.4886 (3)	0.43006 (10)	0.0404 (5)
C4	0.1916 (4)	0.3713 (3)	0.43342 (12)	0.0484 (6)
H4	0.0553	0.3732	0.4531	0.058*
C5	0.2558 (5)	0.2533 (3)	0.40765 (12)	0.0490 (6)
H5	0.1635	0.1752	0.4105	0.059*
C6	0.4567 (4)	0.2487 (3)	0.37740 (11)	0.0445 (6)
C7	0.5256 (5)	0.1191 (3)	0.35046 (12)	0.0514 (6)
C8	0.6517 (5)	0.1263 (3)	0.29837 (12)	0.0508 (6)
C9	0.8241 (6)	0.0312 (4)	0.28794 (14)	0.0719 (9)
H9	0.8603	−0.0375	0.3135	0.086*
C10	0.9426 (8)	0.0375 (4)	0.23996 (16)	0.0887 (12)
H10	1.0606	−0.0259	0.2337	0.106*
C11	0.8877 (8)	0.1367 (4)	0.20143 (15)	0.0836 (11)
H11	0.9675	0.1398	0.1690	0.100*
C12	0.5958 (4)	0.3649 (3)	0.37511 (11)	0.0469 (6)
H12	0.7313	0.3628	0.3551	0.056*
C13	0.5376 (4)	0.4835 (3)	0.40180 (11)	0.0466 (6)
H13	0.6359	0.5595	0.4009	0.056*
C14	0.7176 (8)	0.2303 (4)	0.21048 (13)	0.0751 (10)
H14	0.6798	0.2970	0.1841	0.090*
C15	0.6003 (6)	0.2264 (3)	0.25880 (12)	0.0612 (8)
H15	0.4853	0.2917	0.2650	0.073*

C12–C13 are 1.433(3), 1.220(3) and 1.377(4) *Å* respectively, which are in normal range [16]. A comparison of the corresponding torsion angle of 121.32° in the molecular structure of benzophenone [17], showed that the torsion angle of C15–C8–C7–C6 36.005° in the title structure is relatively small. In molecular packing, non-classical hydrogen bond was observed as following: C14–H14···O2 (d(H14···O2) = 2.60 Å.

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