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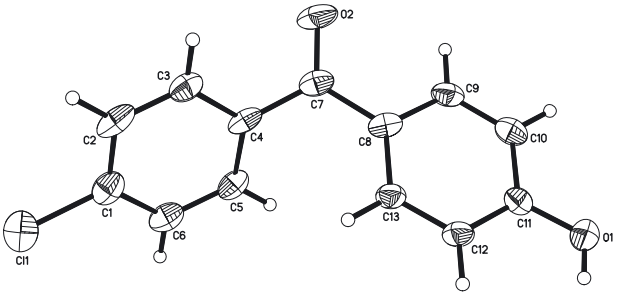
Crystal structure of (4-chlorophenyl)(4-hydroxyphenyl)methanone, $C_{13}H_9ClO_2$



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Abstract

$C_{13}H_9ClO_2$, monoclinic, $P2_1$ (No. 4), a = 6.5465(9) Å, b = 8.0647(11) Å, c = 10.8476(15) Å, β = 105.591(3)°, V = 551.63(13) Å^3, Z = 2, $R_{gt}(F)$ = 0.0532, $wR_{ref}(F^2)$ = 0.1507, T = 296(2) K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

All chemical solvents and reagents are purchased and used without further purification. A mixture of thiophene-2-carbohydrazide (1 mmol, 142.2 mg) and 4-chloro-4′-hydroxybenzophenone (1 mmol, 232.7 mg) in anhydrous ethanol (10 mL) containing a few drops of glacial acetic acid, was refluxed for 2 h, then filtered, left quietly, and evaporated naturally. After three days, colorless block crystals of 4-chloro-4′-hydroxybenzophenone were obtained unexpectedly.

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.25 × 0.20 × 0.18 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.33 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	2796, 1690, 0.025
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1253
$N(param)_{refined}$:	146
Programs:	Bruker programs [1], SHELX [2]

Experimental details

All H atoms were included in calculated positions and refined as riding atoms, with C–H = 0.93 Å and O–H = 0.82 Å. The U_{iso} values were set to be $1.5U_{eq}$(O) and $1.2U_{eq}$(C).

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

Atom	x	y	z	U_{iso}*/U_{eq}
O1	0.8358 (7)	1.0726 (5)	0.5728 (4)	0.0618 (14)
H1	0.756229	1.146993	0.582516	0.093*
O2	0.6388 (8)	0.3264 (6)	0.6637 (5)	0.0735 (15)
Cl1	−0.0012 (3)	0.3639 (3)	1.04651 (18)	0.0822 (7)
C1	0.1700 (9)	0.3902 (8)	0.9494 (6)	0.0567 (17)
C2	0.1450 (10)	0.2919 (7)	0.8390 (6)	0.0609 (19)
H2	0.038138	0.212591	0.818033	0.073*
C3	0.2789 (10)	0.3140 (7)	0.7628 (6)	0.0532 (16)
H3	0.264049	0.248080	0.690608	0.064*
C4	0.4361 (9)	0.4334 (7)	0.7923 (6)	0.0491 (16)
C5	0.4599 (10)	0.5292 (7)	0.9022 (6)	0.0539 (17)
H5	0.565132	0.609892	0.922246	0.065*
C6	0.3283 (10)	0.5058 (8)	0.9823 (7)	0.0586 (18)
H6	0.347685	0.567569	1.056967	0.070*
C7	0.5786 (9)	0.4515 (8)	0.7077 (6)	0.0512 (16)
C8	0.6442 (9)	0.6177 (8)	0.6756 (6)	0.0486 (15)
C9	0.8213 (10)	0.6349 (8)	0.6281 (6)	0.0530 (17)
H9	0.898507	0.541350	0.618271	0.064*
C10	0.8825 (10)	0.7867 (9)	0.5959 (6)	0.0534 (17)
H10	1.002962	0.796166	0.566481	0.064*
C11	0.7668 (9)	0.9266 (8)	0.6068 (5)	0.0459 (15)
C12	0.5876 (9)	0.9116 (8)	0.6493 (6)	0.0496 (15)
H12	0.506712	1.004984	0.654059	0.059*
C13	0.5277 (9)	0.7598 (7)	0.6846 (6)	0.0462 (15)
H13	0.407997	0.751506	0.714936	0.055*

Discussion

As a class of important organic compounds, phenylmethanones have various biological activities such as antifungal, antiinflammatory, antibacterial, and anticancer activities [3–10]. Different substituents in the benzophenone nucleus are essential in investigation of the quantitative structure-activity relationships.

The asymmetric unit of the title compound consists of one formula unit (*cf*. the figure). Crystal determination exhibits that the title compound is monoclinic, $P2_1$ (No. 4), a = 6.5465(9) Å, b = 8.0647(11) Å, c = 10.8476(15) Å, β = 105.591(3)°, V = 551.63(13) Å^3, and Z = 2, which is different from the previously reported the structure of 4-chloro-4′-hydroxybenzophenone determined at 120(2) K, in which of orthorhombic space group $Pca2_1$ (No. 29) with a = 23.3058(11) Å, b = 5.5770(2) Å, c = 8.2847(4) Å, V = 1076.82(8) Å^3, and Z = 4 [10]. In the crystal structure, the short distance d(C7–O2) = 1.225(8) Å exhibits a typical C=O double bond which is not affected by hydrogen bonding. The distance d(C11–O1) = 1.347(7) Å shows a typical C–O single bond. The dihedral angle formed by the two aromatic rings is 55.55(1)°, which is quite different from the literature known structure of 64.66(8)° [10]. In the crystal structure, the molecules are linked into one-dimensional chains along the b-axis direction by O–H···O hydrogen bonds.

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

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