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3-(2,4-Dichlorophenyl)-3-hydroxy-1-(3-nitrophenyl)propan-1-one

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The title compound, $C_{15}H_{11}Cl_2NO_4$, has been synthesized and characterized by single-crystal X-ray diffraction analysis. All bond lengths and angles are within normal ranges. The dihedral angle between the two benzene rings is 77.2 (2)°.

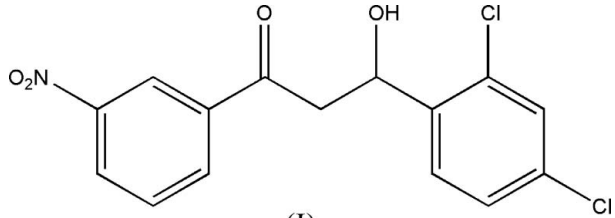
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.063
wR factor = 0.153
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Recently, we have reported a few chalcone derivatives (Qiu, Fang *et al.*, 2006; Qiu, Liu *et al.*, 2006; Qiu, Luo *et al.*, 2006). As an extension of our work on the structural characterization of chalcone derivatives, we report here the structure of the title compound, (I). A view of (I) with the atom-numbering scheme is given in Fig. 1. In (I), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the two benzene rings is 77.2 (2)°. The crystal structure is stabilized by hydrogen bonds (Table 1).



(I)

Experimental

The reagents were commercial products and were used without further purification. An aqueous solution of potassium hydroxide (5%, 1 ml) was added with stirring overnight to a solution of 2,4-dichlorobenzaldehyde (1 mmol, 0.18 g) and 1-(3-nitrophenyl)ethanone (1 mmol, 0.17 g) in ethanol (15 ml) at room temperature. The reaction mixture was then poured into ice and neutralized with hydrochloric acid (5%). A yellow solid was obtained from ethanol. The solid was dissolved in acetone (12 ml) and stirred for about 10 min to give a clear yellow solution. After keeping the solution in air for 9 d, yellow block-shaped crystals were formed at the bottom of the vesssl on slow evaporation of the solvent. These were collected, washed three times with acetone and dried in a vacuum desiccator using $CaCl_2$. The compound was isolated in 65% yield.

Crystal data

$C_{15}H_{11}Cl_2NO_4$
M_r = 340.15
Triclinic, $P\overline{1}$
a = 7.4440 (15) Å
b = 8.5460 (17) Å
c = 12.257 (3) Å
α = 77.86 (3)°
β = 81.28 (3)°
γ = 83.18 (3)°
V = 750.4 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 298 (2) K
0.30 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.945, T_{max} = 0.954
3184 measured reflections
2945 independent reflections
1683 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.153
S = 1.03
2945 reflections
203 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H10···O3^{i}	0.97 (5)	1.89 (5)	2.852 (4)	171 (4)
C8—H7*B*···O1^{ii}	0.97	2.56	3.474 (4)	157
C9—H9···Cl1	0.98	2.67	3.042 (4)	103
C12—H12···O4^{iii}	0.93	2.45	3.275 (4)	148
C14—H14···O3^{ii}	0.93	2.52	3.340 (4)	147
C15—H15···O4	0.93	2.50	2.816 (4)	100

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $x, y+1, z$; (iii) $x+1, y, z$.

H atoms of the CH and CH_2 groups in (I) were positioned geometrically and treated as riding with C—H distances of 0.93–0.98 Å and with U_{iso}(H) = 1.2U_{eq}(C). The H atom of the OH group was located in a difference Fourier map and refined freely.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL*.

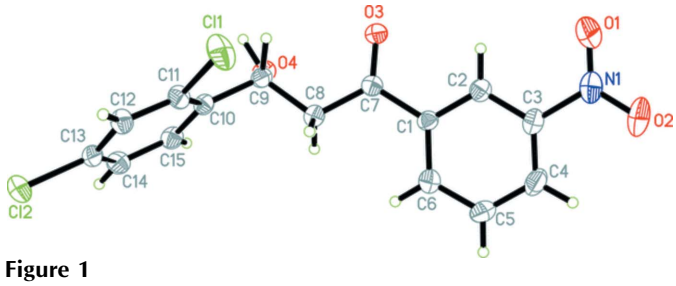


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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