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2,2′,4′-Trichloroacetophenone

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.116
Data-to-parameter ratio = 14.7

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

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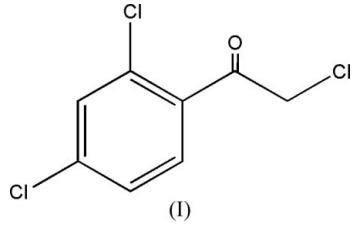
π–π Stacking interactions are present in the crystal structure of the title compound, $C_8H_5Cl_3O$ [systematic name: chloromethyl 2,4-dichlorophenyl ketone].

Comment

2-Substituted acetophenones are often intermediates in the preparation of 1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazines (Demchenko *et al.*, 2003), which exhibit a wide spectrum of biological activity. Acetophenone derivatives have been used for the treatment of diarrhea, coughs, asthma, sores, ulcers, itchy skin, scales, pain and rheumatism, and also have antipyretic, antihemorrhagic, reputed aphrodisiac (Chung *et al.*, 2003) and antifungal activities (Rodriguez *et al.*, 1999). In this paper, we report the synthesis and crystal structure of the title compound, (I).



(I)

In the molecule of (I) (Fig.1), the planarity of the substituted phenyl ring (C1–C6) is unaffected by the chloro substituents. The bond lengths and angles are similar to those in other acetophenones. The C—Cl, C—C, C═O bond lengths [C1—Cl1 = 1.732 (3) Å, C3—Cl12 = 1.735 (3) Å, C8—Cl3 = 1.763 (3) Å, C7—C8 = 1.502 (5) Å, C7—C4 = 1.487 (4) Å and C7═O1 = 1.203 (4) Å] are within normal ranges for acetophenones.

Experimental

The title compound, (I), was synthesized from 2′,4′-dichloroacetophenone (0.01 mol, 1.890 g) and chlorine (0.01 mol) under reflux for 2 h in acetic acid. The desired product was obtained by filtration, drying and recrystallization from ethanol. Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a benzene–toluene (1:2) solution.

Crystal data

$C_8H_5Cl_3O$
M_r = 223.47
Monoclinic, $P2_1/n$
a = 4.6665 (5) Å
b = 10.5576 (11) Å
c = 17.9978 (18) Å
β = 92.299 (2)°
V = 885.98 (16) Å^3
Z = 4
D_x = 1.675 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 298 (2) K
Block, colourless
0.31 × 0.17 × 0.16 mm

Data collection

Bruker APEX area-detector diffractometer	4613 measured reflections
φ and ω scans	1597 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	1415 reflections with $I > 2\sigma(I)$
$T_{min} = 0.752$, $T_{max} = 0.860$	$R_{int} = 0.022$
	$\theta_{max} = 25.2^{\circ}$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 0.8207P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.054$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.116$	$\Delta\rho_{max} = 0.28$ e Å^{-3}
$S = 1.15$	$\Delta\rho_{min} = -0.26$ e Å^{-3}
1597 reflections	
109 parameters	
H-atom parameters constrained	

All H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of Csp^2—H = 0.93 Å and Csp^3—H = 0.97 Å, with U_{iso}(H) = 1.2U_{eq}(parent atom),.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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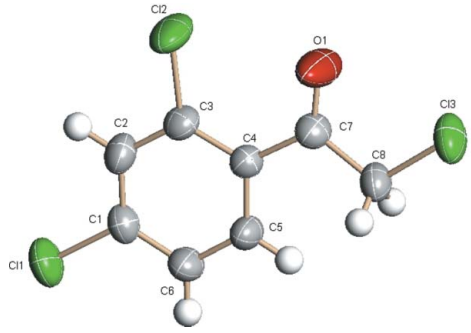

Figure 1
The molecular structure of (I), showing the atom numbering and displacement ellipsoids drawn at the 30% probability level.

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