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Weak C—H···O hydrogen bonding and aromatic π–π-stacking interactions in 1-(4-chlorophenyl)-propan-1-one

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.086
Data-to-parameter ratio = 10.2

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

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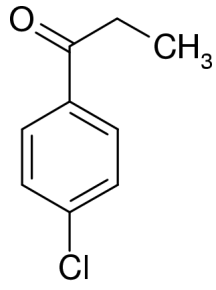
The supramolecular structure of this low melting point compound, C_9H_9ClO, is characterized by weak C—H···O hydrogen bonding and π–π stacking of aromatic rings.

Comment

Propiophenone is a colourless liquid that has been incorporated as a guest into inclusion compounds (Scott, 1997; Gdaniec & Polonski, 1998; Nakano *et al.*, 2001). The 4-chloro derivative, (I), has a low melting point (307–310 K) and has also been subjected to an X-ray crystallographic examination as a guest molecule in an inclusion compound (Weisinger-Lewin *et al.*, 1987). The low melting point suggests that the crystal packing forces are easily broken, and these interactions have been characterized in this investigation.



(I)

The short c axis [3.945 (4) Å] for a disubstituted benzene molecule suggests face-to-face intermolecular π–π-stacking interactions. Mean-plane calculations for the aromatic rings stacked along the c axis give interplanar separations of 3.48 (1) Å (Fig. 2). The rings are displaced from each other (direct overlap is repulsive) such that the shortest separations between any two aromatic C atoms in translation-related rings are C1···C2^{iii} = 3.510 (6) Å and C4···C5^{iii} = 3.511 (6) Å [symmetry code: (iii) x, y, 1+z].

The 16 molecules of the unit cell are shown in Fig. 3. Two weak, but quite linear, C—H···O hydrogen bonds are present (Table 2), such that each molecule is linked to four other molecules (Fig. 4). Here, O1 is the acceptor atom and C2 and C8 are the donor atoms.

The $C_{aromatic}$—Cl bond length [1.747 (3) Å] is normal, as are all other bond lengths and angles for this type of molecule. The shortest intermolecular distance involving the Cl atom is Cl1···C9^{iv} = 3.541 (5) Å [symmetry code: (iv) 5/4−x, −1/4+y, 3/4+z], similar to the sum of van der Waals radii, 3.45 Å (Bondi, 1964; Spek, 2001).

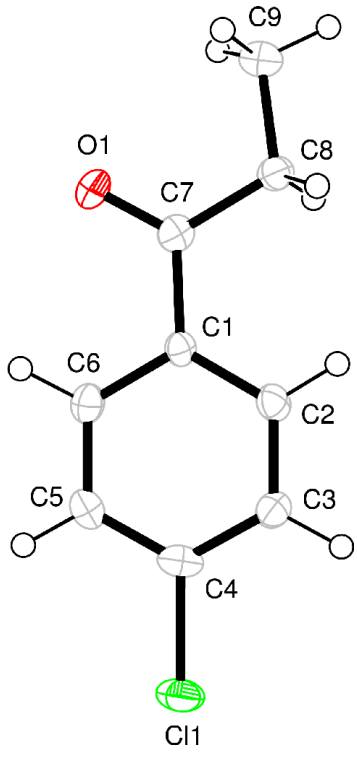


Figure 1
The atomic arrangement in the molecule. Displacement ellipsoids are shown at the 50% probability level.

Experimental

The title compound was purchased from Aldrich and crystals were grown by sublimation.

Crystal data

C_9H_9ClO
M_r = 168.61
Orthorhombic, *Fdd*2
a = 18.6188 (14) Å
b = 45.383 (4) Å
c = 3.945 (4) Å
V = 3334 (3) Å^3
Z = 16
D_x = 1.344 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7501 reflections
θ = 2.9–27.5°
μ = 0.39 mm^{-1}
T = 120 (2) K
Block, colourless
0.20 × 0.10 × 0.08 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.926, T_{max} = 0.969
4434 measured reflections
1292 independent reflections
1105 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
θ_{max} = 27.5°
$h = -23 \rightarrow 24$
$k = -58 \rightarrow 58$
$l = -2 \rightarrow 5$

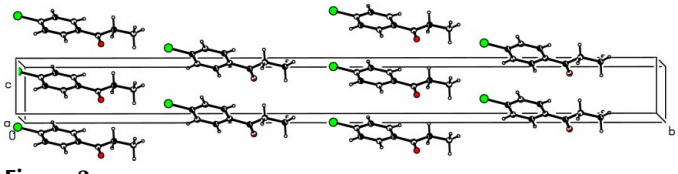


Figure 2
Translation π–π stacking (for clarity, only four of the 16 molecules in the unit cell are utilized).

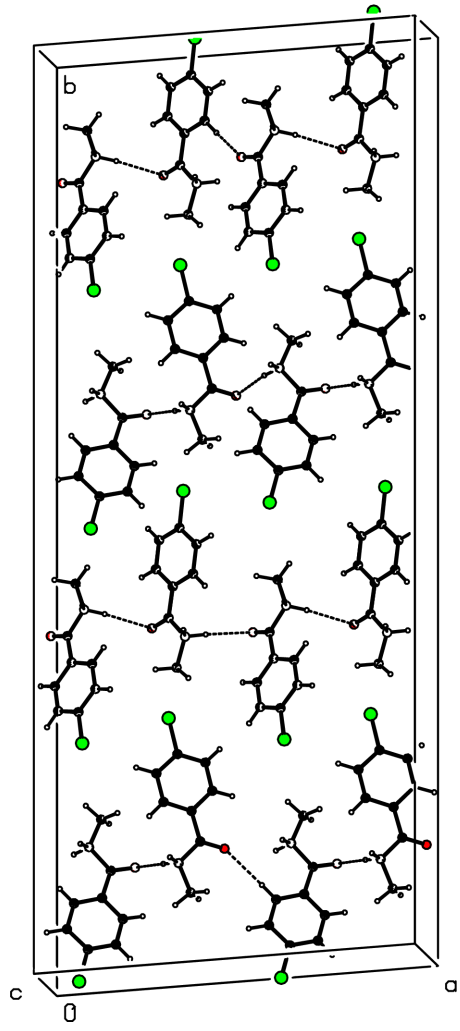


Figure 3
A selection of C—H···O hydrogen bonding between the 16 molecules of the unit cell (additional molecular translations along [001] are required for completeness).

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.086
S = 1.01
1292 reflections
127 parameters
Only coordinates of H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Absolute structure: Flack (1983); 367 Friedel pairs
Flack parameter = 0.08 (9)

Table 1
Selected geometric parameters (Å, °).

Cl1—C4	1.747 (3)	C5—C6	1.376 (4)
O1—C7	1.215 (3)	C7—C8	1.511 (4)
C1—C6	1.403 (4)	C8—C9	1.516 (4)
C1—C7	1.500 (4)		
C7—C8—C9	114.0 (2)		
O1—C7—C8—C9	−6.5 (5)	C1—C7—C8—C9	173.3 (3)

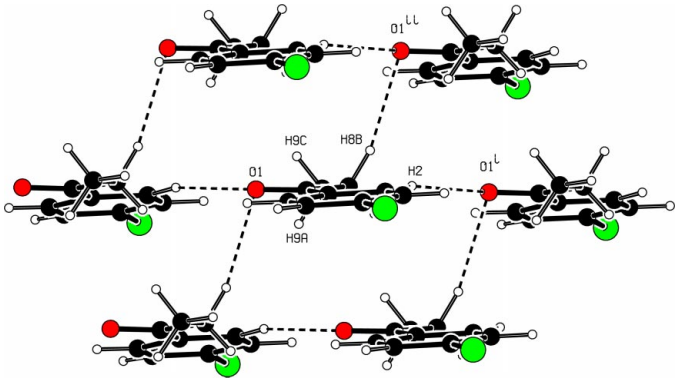


Figure 4
Edge view showing the C—H···O hydrogen bonding linking a 4-chloropropiophenone molecule to four adjacent molecules.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.97 (3)	2.46 (3)	3.404 (5)	167 (3)
C8—H8*B*···O1^{ii}	1.00 (3)	2.48 (3)	3.462 (5)	167 (3)

Symmetry codes: (i) $x-\frac{1}{4},\frac{1}{4}-y,\frac{3}{4}+z$; (ii) $x-\frac{1}{4},\frac{1}{4}-y,z-\frac{1}{4}$.

All H atoms were initially placed in calculated positions and thereafter allowed to refine freely with constrained isotropic displacement parameters; for methyl H atoms $U_{iso} = 1.3U_{eq}$(C), for non-methyl H atoms $U_{iso} = 1.2U_{eq}$(C). Final C—H bond lengths ranged from 0.90 (4) to 1.01 (3) Å.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *PLATON* (Spek, 2001).

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