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Structure of 4-Chlorochalcone

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Abstract

The title compound, 3-(4-chlorophenyl)-1-phenyl-2-propen-1-one, $C_{15}H_{11}ClO$, has a torsion angle of 7.1° for O(1)—C(9)—C(8)—C(7) of the 2-propen-1-one moiety. H atoms in the central propenone group are *trans* and the dihedral angle between the phenyl rings is 14.34°.

Comment

The final atomic coordinates and thermal parameters are given in Table 1, bond lengths and angles are listed in Table 2 and several least-squares planes are given in Table 3. The molecular configuration and the packing of molecules in unit cell are shown in Figs. 1 and 2, respectively.

The torsion angle for O(1)—C(9)—C(8)—C(7) of the C_2H_2CO group is 7.1°. The H atoms are *trans* in the —C=C— part. The dihedral angles between phenyl rings and O(1)—C(9)—C(8)—C(7) are 14.3, 16.3 and 12.3°, respectively. It is significant that conjugation in the title compound is better than in 4-bromochalcone (Li, Pa & Su, 1992).

The chalcone derivatives are newly developed organic crystals with nonlinear optical coefficients (Fichou, Watanabe, Takeda, Miyata, Goto & Nakayama, 1988). In order to explore the relationship between their structure and nonlinear optical properties, we synthesized a series of substituted chalcones. The title compound is one of them, which happens to crystallize in a centrosymmetric space group and therefore has no nonlinear optical properties. This has been confirmed by second harmonic generation (SHG) efficiency measurements on a powder sample using the method of Kurtz & Perry (1968).

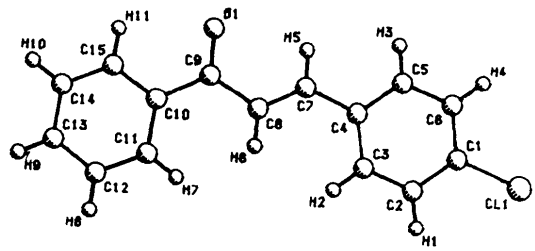

Fig. 1. The molecular structure of the title compound.

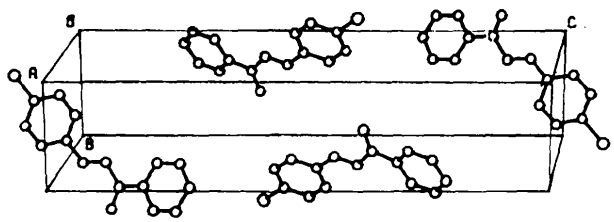

Fig. 2. The packing of the title compound in the unit cell.

Experimental

Crystal data

$C_{15}H_{11}ClO$
M_r = 242.70
Monoclinic
$P2_1/c$
a = 8.211 (2) Å
b = 5.869 (2) Å
c = 25.291 (5) Å
β = 99.18°
V = 1203.1 (5) Å^3
Z = 4
D_x = 1.340 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 20 reflections
θ = 6.5–11°
μ = 0.293 mm^{-1}
T = 294 K
Plate
1.0 × 0.5 × 0.1 mm
Colourless

Data collection

Rigaku MSC/AFC-5*R* diffractometer
ω-2θ scans
Absorption correction: empirical based on ψ scans (*DIFABS*; Walker & Stuart, 1983)
T_{min} = 0.737, T_{max} = 1.341
2498 measured reflections
2328 independent reflections
1264 observed reflections [$I > 3\sigma(I)$]
θ_{max} = 25°
h = 0 → 10
k = 0 → 7
l = −30 → 30
3 standard reflections monitored every 250 reflections
intensity variation: 0.1%

Refinement

Refinement on F	$(\Delta/\sigma)_{max} = 0.01$
$R = 0.045$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
$wR = 0.054$	$\Delta\rho_{min} = -0.18$ e Å^{-3}
$S = 1.36$	Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)
1264 reflections	
154 parameters	
$w = 1/\sigma^2(F_o)$	
Extinction correction: none	

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = \frac{4}{3}\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
Cl(1)	0.5320 (1)	0.1672 (2)	−0.09416 (4)	5.73 (5)
O(1)	1.0844 (3)	1.1110 (4)	0.1345 (1)	5.9 (1)
C(1)	0.6451 (4)	0.3432 (5)	−0.0466 (1)	3.9 (1)
C(2)	0.6741 (4)	0.2757 (5)	0.0065 (1)	4.3 (1)
C(3)	0.7644 (4)	0.4137 (6)	0.0440 (1)	4.2 (1)
C(4)	0.8238 (3)	0.6239 (5)	0.0299 (1)	3.7 (1)
C(5)	0.7914 (4)	0.6856 (5)	−0.0238 (1)	4.2 (1)
C(6)	0.7040 (4)	0.5474 (6)	−0.0620 (1)	4.4 (2)
C(7)	0.9177 (4)	0.7774 (5)	0.0686 (1)	4.2 (1)
C(8)	0.9860 (4)	0.7378 (6)	0.1183 (1)	4.2 (1)
C(9)	1.0806 (4)	0.9151 (6)	0.1512 (1)	4.1 (1)
C(10)	1.1723 (4)	0.8585 (5)	0.2050 (1)	3.8 (1)
C(11)	1.1522 (4)	0.6557 (6)	0.2318 (1)	4.8 (2)
C(12)	1.2366 (5)	0.6188 (7)	0.2826 (1)	5.8 (2)
C(13)	1.3430 (5)	0.7795 (8)	0.3072 (1)	6.0 (2)
C(14)	1.3679 (5)	0.9797 (7)	0.2809 (2)	6.4 (2)
C(15)	1.2821 (5)	1.0178 (6)	0.2307 (1)	5.2 (2)

Table 2. *Geometric parameters* (Å, °)

Cl(1)—C(1)	1.737 (3)	C(7)—C(8)	1.313 (4)
O(1)—C(9)	1.227 (4)	C(8)—C(9)	1.474 (4)
C(1)—C(6)	1.372 (4)	C(9)—C(10)	1.484 (4)
C(1)—C(2)	1.384 (4)	C(10)—C(15)	1.387 (4)
C(2)—C(3)	1.371 (4)	C(10)—C(11)	1.392 (4)
C(3)—C(4)	1.393 (4)	C(11)—C(12)	1.375 (5)
C(4)—C(5)	1.390 (4)	C(12)—C(13)	1.366 (5)
C(4)—C(7)	1.457 (4)	C(13)—C(14)	1.382 (5)
C(5)—C(6)	1.374 (4)	C(14)—C(15)	1.367 (5)
C(6)—C(1)—C(2)	120.8 (3)	O(1)—C(9)—C(8)	120.4 (3)
C(6)—C(1)—Cl(1)	119.7 (2)	O(1)—C(9)—C(10)	119.2 (3)
C(2)—C(1)—Cl(1)	119.5 (3)	C(8)—C(9)—C(10)	120.3 (3)
C(3)—C(2)—C(1)	119.5 (3)	C(15)—C(10)—C(11)	117.9 (3)
C(2)—C(3)—C(4)	121.3 (3)	C(15)—C(10)—C(9)	118.4 (3)
C(5)—C(4)—C(3)	117.4 (3)	C(11)—C(10)—C(9)	123.7 (3)
C(5)—C(4)—C(7)	119.5 (3)	C(12)—C(11)—C(10)	120.5 (3)
C(3)—C(4)—C(7)	123.1 (3)	C(13)—C(12)—C(11)	120.5 (3)
C(6)—C(5)—C(4)	122.1 (3)	C(12)—C(13)—C(14)	120.0 (3)
C(1)—C(6)—C(5)	118.9 (3)	C(15)—C(14)—C(13)	119.5 (3)
C(8)—C(7)—C(4)	129.2 (3)	C(14)—C(15)—C(10)	121.6 (3)
C(7)—C(8)—C(9)	121.5 (3)		

Table 3. *Selected least-squares planes*

Plane 1

Atoms defining plane	Distance (Å)	E.s.d.
Cl(1)	−0.0003	0.0009
C(1)	0.0036	0.0030
C(2)	−0.0042	0.0032
C(3)	0.0088	0.0032
C(4)	−0.0063	0.0029
C(5)	−0.0038	0.0031
C(6)	0.0102	0.0034
Additional atoms		
C(7)	−0.0158	
C(8)	0.2123	
C(9)	0.1886	
O(1)	−0.1729	

Mean deviation from plane 0.0053 Å, $\chi^2 = 33.9$

Plane 2

Atoms defining plane	Distance (Å)	E.s.d.
C(10)	−0.0063	0.0030
C(11)	0.0086	0.0033
C(12)	−0.0026	0.0039
C(13)	−0.0098	0.0043
C(14)	0.0088	0.0040
C(15)	−0.0007	0.0035
Additional atoms		
C(7)	0.2830	
C(8)	0.1845	
C(9)	−0.0552	
O(1)	−0.2915	

Mean deviation from plane 0.0061 Å, $\chi^2 = 18.9$

Plane 3

Atoms defining plane	Distance (Å)	E.s.d.
C(7)	−0.0148	0.0030
C(8)	−0.0294	0.0032
C(9)	0.0294	0.0031
O(1)	−0.0088	0.0024
Additional atoms		
C(4)	−0.0013	
C(10)	0.1326	

Mean deviation from plane 0.0206 Å, $\chi^2 = 219.9$

Dihedral angles between least-squares planes

Plane	Plane	Angle (°)
2	1	14.34
3	1	16.32
3	2	12.28

The title compound was prepared by the acyloin condensation method from 4-chlorobenzaldehyde and acetophenone at room temperature (Migrdichian, 1957). The crystals were obtained from ethanol, then mounted on a glass fibre in a random orientation. Lattice parameters were determined by least-squares techniques and the data corrected for Lorentz and polarization factors. The structure was solved by direct methods; H-atom coordinates were added according to theoretical models and included in the structure-factor calculations. The scale-factor and positional and thermal parameters for the non-H atoms were refined by full-matrix least-squares techniques, the function minimized being $\Sigma w(|F_o|-|F_c|)^2$. All calculations were performed on a VAX computer using the *TEXSAN* crystallographic software package (Molecular Structure Corporation, 1985).

Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71397 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR1057]

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