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(2*E*)-3-(Biphenyl-4-yl)-1-(2,4-dichlorophenyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.050
wR factor = 0.106
Data-to-parameter ratio = 13.4

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

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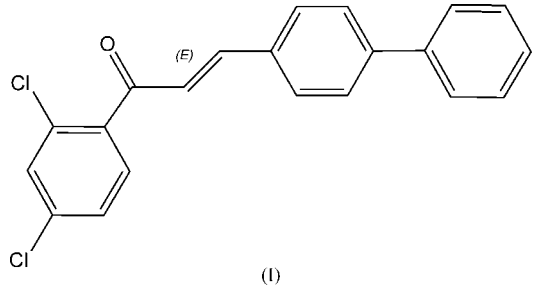
The title compound, $C_{21}H_{14}Cl_2O$, was prepared from biphenyl-4-carbaldehyde and 2,4-dichloroacetophenone. Single crystals were obtained from acetone. The compound crystallizes with four molecules in the asymmetric unit, all of which deviate significantly from planarity.

Comment

For an introduction, see Fischer *et al.* (2007).



(I)

Fig. 1 shows the four molecules in the asymmetric unit of the title compound, (I). All molecules deviate significantly from planarity; Table 1 provides values for the dihedral angles.

Experimental

2,4-Dichloroacetophenone (1.89 g, 0.01 mol) in methanol (20 ml) was mixed with biphenyl-4-carbaldehyde (1.82 g, 0.01 mol) and the mixture was treated with a 30% potassium hydroxide solution (3 ml) at 278 K. The reaction mixture was then brought to room temperature and stirred for 3 h. The precipitated solid was filtered off, washed with water, dried and recrystallized from acetone (m.p. 396–398 K). Analysis (%) for $C_{21}H_{14}Cl_2O$ found (calculated): C 71.31 (71.40), H 3.86 (3.99).

Crystal data

$C_{21}H_{14}Cl_2O$
M_r = 353.25
Triclinic, $P\overline{1}$
a = 7.6022 (6) Å
b = 11.9149 (14) Å
c = 37.877 (4) Å
α = 85.413 (8)°
β = 85.375 (6)°
γ = 86.547 (7)°
V = 3403.7 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 296 K
0.60 × 0.53 × 0.23 mm

Data collection

Bruker-Nonius KappaCCD diffractometer
Absorption correction: numerical (Herrendorf & Bärnighausen, 1997)
T_{min} = 0.810, T_{max} = 0.911
30533 measured reflections
11578 independent reflections
7410 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

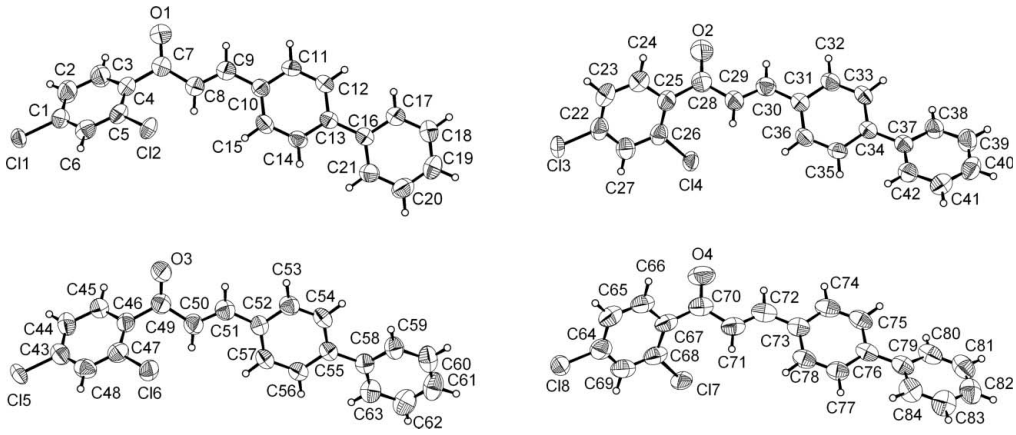


Figure 1
The molecular structure of the four molecules in the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level.

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$	866 parameters
$wR(F^2) = 0.106$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{max} = 0.24$ e Å^{-3}
11578 reflections	$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Dihedral angles (°) within biphenyl groups and between biphenyl and dichlorophenyl groups..

Molecule	Dihedral angle (biphenyl)	Dihedral angle (biphenyl/dichlorophenyl)
a	17.67 (7)	41.42 (9)
b	24.52 (8)	40.42 (9)
c	18.91 (7)	61.13 (9)
d	24.17 (9)	54.5 (1)

Notes: for the calculation of the dihedral angle between the biphenyl group and the dichlorophenyl group, a least-squares plane through the atoms of the nearer phenyl group was calculated. Molecule *a* contains atoms from Cl1 to H21, molecule *b* contains atoms from Cl3 to H42, molecule *c* contains atoms from Cl5 to H63 and molecule *d* contains atoms from Cl7 to H84.

All H atoms were placed at calculated positions and refined as riding on the respective carrier atom, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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