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(2*E*,2′*E*)-1,1′-Bis(4-chlorophenyl)-3,3′-(1,4-phenylene)diprop-2-en-1-one

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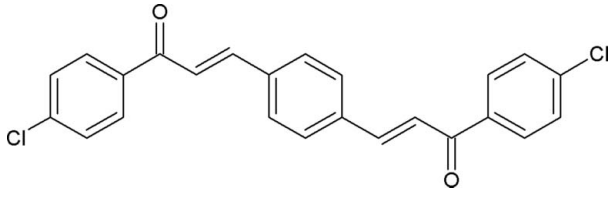
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.005 Å; R factor = 0.061; wR factor = 0.200; data-to-parameter ratio = 13.7.

In the centrosymmetric title compound, $C_{24}H_{16}Cl_2O_2$, the dihedral angle between the central and terminal benzene rings is 46.27 (9)°. Edge-to-face C—H···π interactions are observed, with H···centroid distances in the range 2.70–2.83 Å. Cl···Cl contacts of 3.3701 (14) Å are also present.

Related literature

For related structures, see: Harrison *et al.* (2007*a*,*b*).



Experimental

Crystal data

$C_{24}H_{16}Cl_2O_2$
M_r = 407.26
Monoclinic, $P2_1/c$
a = 22.9779 (19) Å
b = 7.0369 (5) Å
c = 5.8425 (5) Å
β = 95.229 (3)°
V = 940.76 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 120 (2) K
0.24 × 0.12 × 0.02 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.918, T_{max} = 0.993
6340 measured reflections
1739 independent reflections
1556 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.200
S = 1.16
1739 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C3/C1^{i}–C3^{i} ring and *Cg*2 is the centroid of the C7–C12 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···*Cg*1^{ii}	0.95	2.70	3.400 (3)	131
C9—H9···*Cg*2^{iii}	0.95	2.77	3.422 (4)	127
C12—H12···*Cg*2^{iv}	0.95	2.83	3.457 (3)	124

Symmetry codes: (i) $-x, 1-y, -z$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997), and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2226).

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supplementary materials

Acta Cryst. (2007). E**63**, o3702 [**doi:10.1107/S1600536807037634**]

(2*E*,2'*E*)-1,1'-Bis(4-chlorophenyl)-3,3'-(1,4-phenylene)diprop-2-en-1-one

W. T. A. Harrison, H. J. Ravindra, M. R. S. Kumar and S. M. Dharmaprakash

Comment

As part of our ongoing studies of organic nonlinear optical materials derived from substituted chalcones (Harrison *et al.*, 2007*a*,*b*), we report here the synthesis and structure of the title compound (Fig. 1).

The molecule is centrosymmetric and the dihedral angle between the mean planes of the central C1–C3/C1^{i}–C3^{i} [symmetry code: (i) −*x*, 1 − *y*, −*z*] and pendant C7–C12 benzene rings is 46.27 (9)°. The linking enone (C4/C5/C6/O1) fragment is substantially twisted, with a torsion angle of −19.3 (5)°.

In the crystal, the molecules lie in sheets in the (100) planes, with C—H···π interactions observed between molecules (Table 1, Figs. 2 and 3). Inter-sheet Cl1···Cl1^{ii} contacts [symmetry code: (ii) 1 − *x*, 1 − *y*, −*z*] of 3.3701 (14)Å are formed, which are slightly short compared to the expected van der Waals separation of 3.50 Å.

Experimental

A mixture of methanol (25 ml) and 10% aqueous NaOH (5 ml) solution were taken in a conical flask. A previously prepared small portion of terephthalaldehyde (0.001 mol) and 1-(4-chlorophenyl)ethanone (0.002 mol) dissolved in methanol was added to the conical flask with stirring and the temperature of the solution was maintained between 298 and 303 K. A precipitate was obtained after stirring the solution for about five minutes. The remaining portion of the aldehyde and ketone mixture was added and the solution was stirred for a further 60 minutes. The separated product was filtered, washed with water and dried. The resulting compound was purified by recrystallization from DMF. Single crystals used for X-ray diffraction analysis were grown by slow evaporation of a DMF solution.

Refinement

H atoms were placed in calculated positions (C—H = 0.95 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

Figures

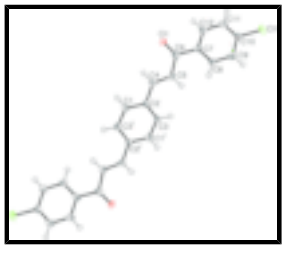

Fig. 1. The molecular structure of the title compound showing 50% displacement ellipsoids (H atoms are drawn as spheres of arbitrary radius). Symmetry code: (i) −*x*, 1 − *y*, −*z*.

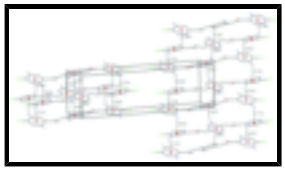

Fig. 2. Partial packing diagram showing the C—H···π interactions as dashed lines.

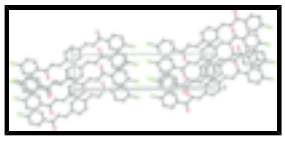

Fig. 3. Unit-cell packing viewed down [010] with H atoms omitted for clarity.

(2*E*,2'*E*)-1,1'-Bis(4-chlorophenyl)-3,3'-(1,4-phenylene)diprop- 2-en-1-one

Crystal data

$C_{24}H_{16}Cl_2O_2$	F_{000} = 420
M_r = 407.26	D_x = 1.438 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8003 reflections
a = 22.9779 (19) Å	θ = 2.9–27.5º
b = 7.0369 (5) Å	μ = 0.36 mm^{-1}
c = 5.8425 (5) Å	T = 120 (2) K
β = 95.229 (3)º	Plate, pale yellow
V = 940.76 (13) Å^3	0.24 × 0.12 × 0.02 mm
Z = 2	

Data collection

Nonius KappaCCD area-detector diffractometer	1739 independent reflections
Radiation source: fine-focus sealed tube	1556 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 120(2) K	θ_{max} = 26.0º
ω and φ scans	θ_{min} = 3.0º
Absorption correction: multi-scan (SADABS; Bruker, 2003)	h = −28→28
T_{min} = 0.918, T_{max} = 0.993	k = −8→8
6340 measured reflections	l = −7→7

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.061	H-atom parameters constrained
$wR(F^2)$ = 0.200	$w = 1/[\sigma^2(F_o^2) + (0.0964P)^2 + 1.6678P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.16	$(\Delta/\sigma)_{max} < 0.001$

1739 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
127 parameters	$\Delta\rho_{min} = -0.45$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.00124 (14)	0.4218 (4)	0.2158 (5)	0.0217 (7)
H1	−0.0022	0.3663	0.3636	0.026*
C2	0.05237 (13)	0.4808 (4)	0.1436 (5)	0.0200 (7)
C3	0.05293 (14)	0.5572 (4)	−0.0756 (6)	0.0220 (7)
H3	0.0889	0.5952	−0.1298	0.026*
C4	0.10477 (14)	0.4691 (4)	0.3076 (6)	0.0229 (7)
H4	0.0995	0.4224	0.4569	0.027*
C5	0.15882 (14)	0.5176 (4)	0.2671 (6)	0.0237 (7)
H5	0.1668	0.5538	0.1164	0.028*
C6	0.20686 (15)	0.5159 (4)	0.4554 (6)	0.0246 (7)
C7	0.26819 (14)	0.5103 (4)	0.3861 (6)	0.0217 (7)
C8	0.28095 (14)	0.4390 (4)	0.1750 (6)	0.0241 (7)
H8	0.2501	0.4002	0.0659	0.029*
C9	0.33836 (15)	0.4239 (5)	0.1218 (6)	0.0264 (7)
H9	0.3471	0.3707	−0.0205	0.032*
C10	0.38278 (14)	0.4877 (5)	0.2800 (6)	0.0249 (7)
C11	0.37131 (15)	0.5624 (5)	0.4894 (6)	0.0282 (8)
H11	0.4023	0.6067	0.5947	0.034*
C12	0.31431 (15)	0.5719 (4)	0.5438 (6)	0.0256 (7)
H12	0.3060	0.6205	0.6891	0.031*
O1	0.19730 (10)	0.5193 (4)	0.6579 (4)	0.0313 (6)
Cl1	0.45434 (4)	0.47454 (16)	0.20782 (17)	0.0420 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0257 (15)	0.0183 (14)	0.0209 (15)	−0.0002 (12)	0.0004 (12)	−0.0028 (12)
C2	0.0198 (14)	0.0192 (14)	0.0208 (15)	0.0006 (11)	0.0013 (11)	−0.0028 (12)

C3	0.0188 (14)	0.0203 (14)	0.0270 (16)	−0.0026 (11)	0.0024 (12)	−0.0008 (12)
C4	0.0239 (16)	0.0223 (15)	0.0215 (16)	0.0013 (12)	−0.0025 (13)	−0.0004 (12)
C5	0.0237 (16)	0.0262 (16)	0.0207 (16)	0.0030 (12)	−0.0012 (12)	0.0022 (13)
C6	0.0254 (16)	0.0203 (15)	0.0272 (18)	0.0025 (12)	−0.0034 (13)	−0.0014 (13)
C7	0.0215 (15)	0.0190 (14)	0.0235 (16)	0.0025 (12)	−0.0044 (12)	0.0021 (12)
C8	0.0244 (16)	0.0216 (15)	0.0250 (17)	0.0006 (12)	−0.0047 (13)	−0.0020 (13)
C9	0.0280 (17)	0.0244 (16)	0.0266 (17)	0.0039 (13)	0.0017 (13)	−0.0002 (13)
C10	0.0213 (15)	0.0271 (16)	0.0268 (17)	0.0005 (13)	0.0045 (13)	0.0034 (13)
C11	0.0261 (17)	0.0267 (17)	0.0302 (18)	0.0003 (13)	−0.0062 (14)	0.0018 (14)
C12	0.0312 (17)	0.0197 (15)	0.0245 (16)	0.0007 (12)	−0.0059 (14)	−0.0008 (13)
O1	0.0244 (12)	0.0489 (16)	0.0209 (13)	0.0015 (10)	0.0031 (9)	0.0000 (10)
Cl1	0.0227 (5)	0.0617 (7)	0.0423 (6)	0.0030 (4)	0.0066 (4)	0.0023 (4)

Geometric parameters (Å, °)

C1—C3^{i}	1.388 (4)	C6—C7	1.502 (5)
C1—C2	1.401 (5)	C7—C8	1.387 (5)
C1—H1	0.950	C7—C12	1.408 (4)
C2—C3	1.390 (5)	C8—C9	1.387 (5)
C2—C4	1.471 (4)	C8—H8	0.950
C3—C1^{i}	1.388 (4)	C9—C10	1.388 (5)
C3—H3	0.950	C9—H9	0.950
C4—C5	1.330 (5)	C10—C11	1.379 (5)
C4—H4	0.950	C10—Cl1	1.737 (3)
C5—C6	1.486 (4)	C11—C12	1.377 (5)
C5—H5	0.950	C11—H11	0.950
C6—O1	1.223 (4)	C12—H12	0.950
C3^{i}—C1—C2	121.3 (3)	C8—C7—C12	119.1 (3)
C3^{i}—C1—H1	119.4	C8—C7—C6	121.9 (3)
C2—C1—H1	119.4	C12—C7—C6	119.0 (3)
C3—C2—C1	118.3 (3)	C9—C8—C7	120.6 (3)
C3—C2—C4	123.1 (3)	C9—C8—H8	119.7
C1—C2—C4	118.5 (3)	C7—C8—H8	119.7
C1^{i}—C3—C2	120.4 (3)	C8—C9—C10	118.8 (3)
C1^{i}—C3—H3	119.8	C8—C9—H9	120.6
C2—C3—H3	119.8	C10—C9—H9	120.6
C5—C4—C2	126.3 (3)	C11—C10—C9	121.7 (3)
C5—C4—H4	116.9	C11—C10—Cl1	119.8 (3)
C2—C4—H4	116.9	C9—C10—Cl1	118.4 (3)
C4—C5—C6	120.6 (3)	C12—C11—C10	119.1 (3)
C4—C5—H5	119.7	C12—C11—H11	120.5
C6—C5—H5	119.7	C10—C11—H11	120.5
O1—C6—C5	121.9 (3)	C11—C12—C7	120.6 (3)
O1—C6—C7	121.1 (3)	C11—C12—H12	119.7
C5—C6—C7	116.9 (3)	C7—C12—H12	119.7
C3^{i}—C1—C2—C3	−1.6 (5)	C5—C6—C7—C12	158.7 (3)
C3^{i}—C1—C2—C4	175.0 (3)	C12—C7—C8—C9	1.6 (5)

C1—C2—C3—C1^{i}	1.6 (5)	C6—C7—C8—C9	−175.7 (3)
C4—C2—C3—C1^{i}	−174.8 (3)	C7—C8—C9—C10	−2.3 (5)
C3—C2—C4—C5	−4.1 (5)	C8—C9—C10—C11	1.2 (5)
C1—C2—C4—C5	179.5 (3)	C8—C9—C10—Cl1	−178.1 (2)
C2—C4—C5—C6	174.1 (3)	C9—C10—C11—C12	0.7 (5)
C4—C5—C6—O1	−19.3 (5)	Cl1—C10—C11—C12	180.0 (2)
C4—C5—C6—C7	160.9 (3)	C10—C11—C12—C7	−1.4 (5)
O1—C6—C7—C8	156.2 (3)	C8—C7—C12—C11	0.3 (5)
C5—C6—C7—C8	−24.0 (4)	C6—C7—C12—C11	177.6 (3)
O1—C6—C7—C12	−21.1 (4)		

Symmetry codes: (i) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···Cg1^{ii}	0.95	2.70	3.400 (3)	131
C9—H9···Cg2^{iii}	0.95	2.77	3.422 (4)	127
C12—H12···Cg2^{iv}	0.95	2.83	3.457 (3)	124

Symmetry codes: (ii) −*x*, *y*−1/2, −*z*+1/2; (iii) *x*, −*y*+1/2, *z*−1/2; (iv) *x*, −*y*+3/2, *z*+1/2.

Fig. 1

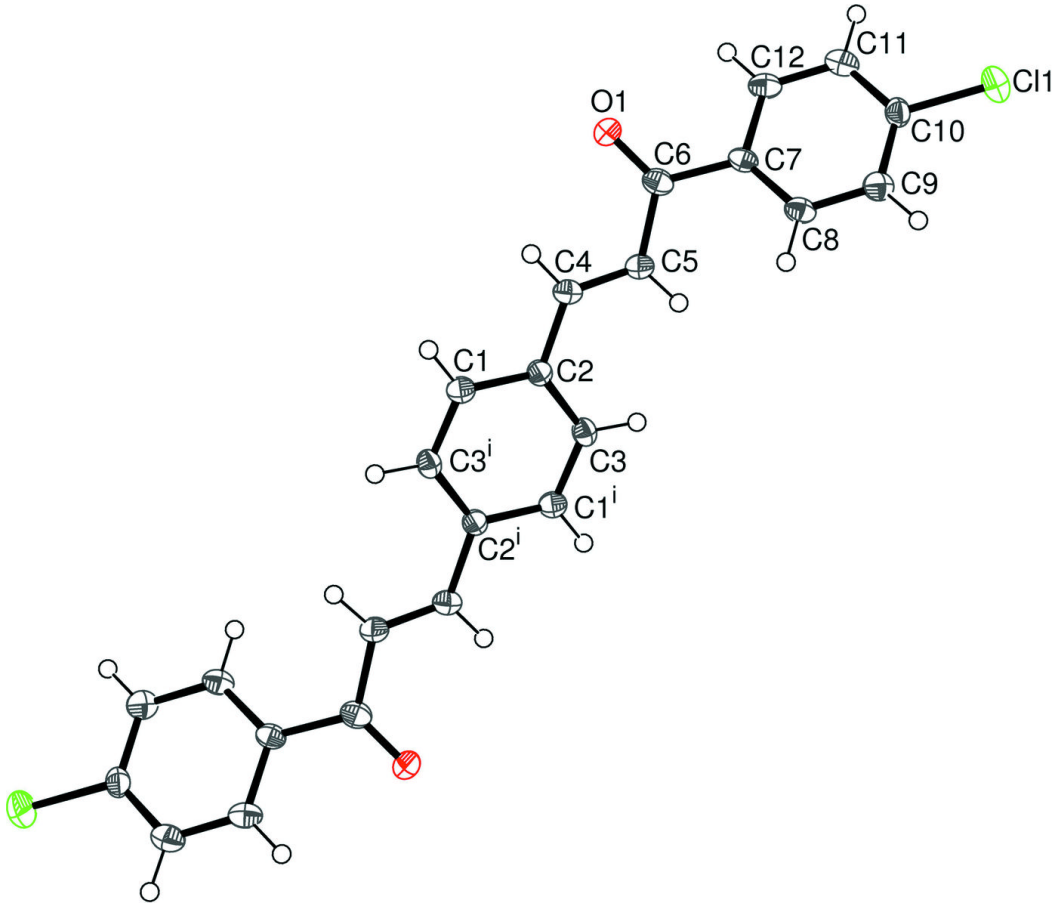

Fig. 2

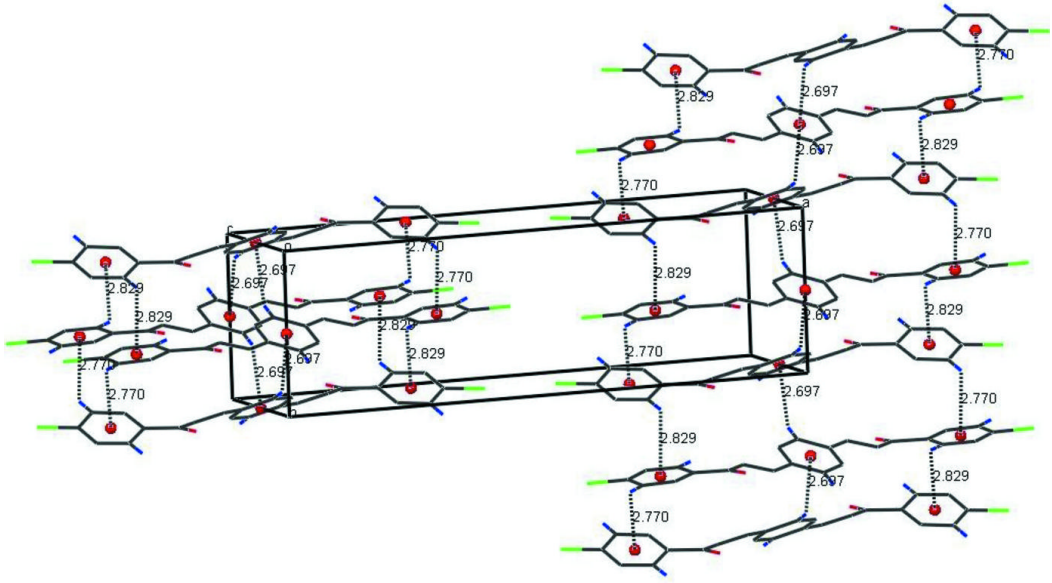
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Fig. 3