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3-[(*E*)-2-(4-Chlorophenyl)ethenyl]-5,5-dimethylcyclohex-2-en-1-one

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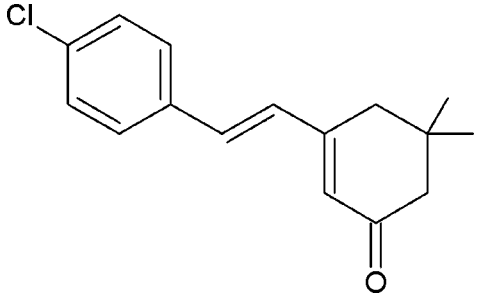
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.130; data-to-parameter ratio = 21.5.

In the title compound, $C_{16}H_{17}ClO$, the cyclohexene ring adopts a half-chair conformation and the best plane through the six ring atoms makes a dihedral angle of 6.69 (7)° with the chlorophenyl ring. In the crystal, pairs of C—H···O hydrogen bonds link the molecules into centrosymmetric $R_2^2(20)$ dimers. The dimers are linked into an infinite chains along the b-axis direction by further C—H···O hydrogen bonds.

Related literature

For the pharmacological activity of cyclohexanone derivatives, see: Puetz *et al.*(2003); Rajveer *et al.* (2010). For a related structure, see: Hema *et al.* (2006). For conformational analysis, see: Allinger (1977); Cremer & Pople (1975).



Experimental

Crystal data

$C_{16}H_{17}ClO$
M_r = 260.75
Monoclinic, $P2_1/n$
a = 13.7630 (4) Å
b = 6.0841 (2) Å
c = 17.5003 (6) Å
β = 105.726 (2)°
V = 1410.54 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 293 K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.927, T_{max} = 0.951
13158 measured reflections
3552 independent reflections
2611 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.130
S = 1.03
3552 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.41	3.301 (2)	159
C14—H14B···O1^{ii}	0.97	2.57	3.4299 (18)	148

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6912).

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supporting information

Acta Cryst. (2013). E**69**, o1121 [https://doi.org/10.1107/S1600536813016255]

3-[(*E*)-2-(4-Chlorophenyl)ethenyl]-5,5-dimethylcyclohex-2-en-1-one

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S1. Comment

Cyclohexanone derivatives have potent pharmacological activity in the treatment of a broad spectrum of medical conditions (Puetz *et al.*, 2003). The cyclohexanone moiety constitutes an important structural feature in several antiinflammatory, analgesic, local anesthetic and antihistaminic drugs (Rajveer *et al.*, 2010). In view of different applications of this class of compounds, we have undertaken a single-crystal structure determination of the title compound.

Molecules of the title compound, $C_{16}H_{17}ClO$, (Fig.1) are linked by pairs of intermolecular (C2—H2···O1) hydrogen bonds (Fig. 2) into centrosymmetric $R_2^2(20)$ dimers and these dimers are linked into an infinite chains by pairs of (C14—H14B···O1) hydrogen bonds, which propagate in the *b* axis direction. The cyclohexene ring (C9—C14) adopts a *half-chair* conformation and makes a dihedral angle of 6.69 (7)° with the phenyl ring (C1—C6).

S2. Experimental

A mixture of isophorone (0.01 mol), 4-chlorobezaldehyde (0.01 mol) and sodium hydroxide solution (10 mL, 10%) in ethanol (25 mL) was stirred at room temperature until the starting material disappeared. The resulting mixture was poured into crushed ice and the precipitate was filtered off, dried and recrystallized from ethanol. Yield=90%, Melting point=84–86°C.

S3. Refinement

The hydrogen atoms were placed in calculated positions with C—H = 0.92 Å to 0.97 Å refined in the riding model with fixed isotropic displacement parameters:U_{iso}(H) = 1.5U_{eq}(C) for methyl group and U_{iso}(H) = 1.2U_{eq}(C) for other groups.

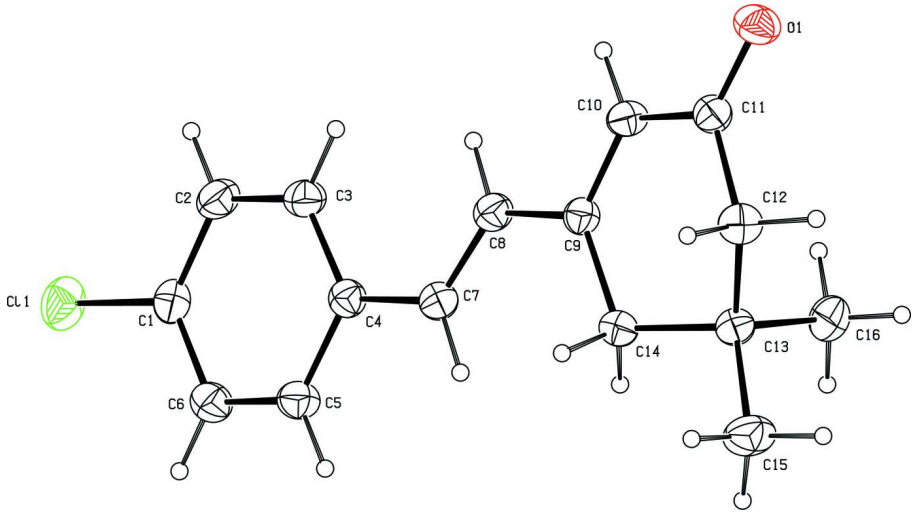

Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radius.

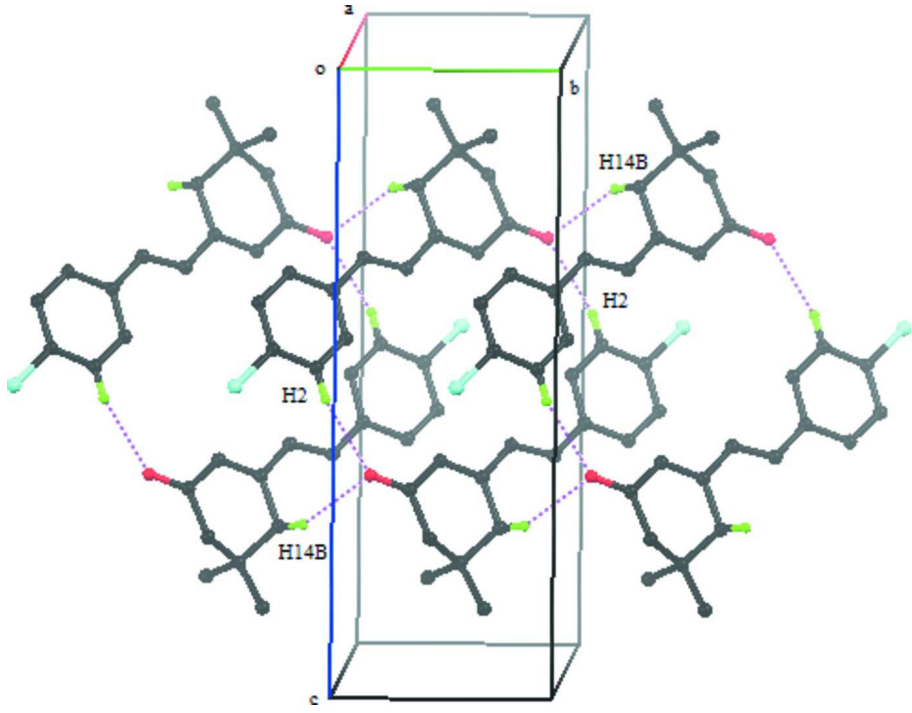

Figure 2

The crystal packing of the title compound viewed down *a* axis. H-atoms not involved in H-bonds have been excluded for clarity.

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Crystal data

$C_{16}H_{17}ClO$
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Monoclinic, $P2_1/n$
$a = 13.7630\ (4)$ Å

b = 6.0841 (2) Å
c = 17.5003 (6) Å
β = 105.726 (2)°
V = 1410.54 (8) Å^3
Z = 4
$F(000)$ = 552
D_x = 1.228 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3552 reflections
θ = 1.7–28.5°
μ = 0.26 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.927, T_{max} = 0.951

13158 measured reflections
3552 independent reflections
2611 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28.5°, θ_{min} = 1.7°
h = −17→18
k = −8→8
l = −21→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.130
S = 1.03
3552 reflections
165 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.2499P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.25679 (10)	−0.3118 (3)	0.46901 (9)	0.0552 (4)
C2	0.30278 (13)	−0.1202 (3)	0.50163 (9)	0.0631 (4)
H2	0.3008	−0.0766	0.5521	0.076*
C3	0.35172 (13)	0.0062 (3)	0.45851 (9)	0.0600 (4)
H3	0.3831	0.1356	0.4807	0.072*
C4	0.35569 (10)	−0.0537 (2)	0.38278 (8)	0.0490 (3)
C5	0.30813 (11)	−0.2484 (3)	0.35197 (9)	0.0572 (4)
H5	0.3095	−0.2927	0.3014	0.069*
C6	0.25905 (12)	−0.3775 (3)	0.39444 (9)	0.0592 (4)
H6	0.2278	−0.5076	0.3729	0.071*

C7	0.40805 (11)	0.0754 (2)	0.33556 (8)	0.0518 (3)
H7	0.4065	0.0202	0.2857	0.062*
C8	0.45744 (11)	0.2628 (2)	0.35633 (8)	0.0531 (3)
H8	0.4574	0.3211	0.4055	0.064*
C9	0.51163 (10)	0.3859 (2)	0.30951 (8)	0.0471 (3)
C10	0.56090 (11)	0.5706 (2)	0.33930 (8)	0.0529 (3)
H10	0.5568	0.6189	0.3887	0.063*
C11	0.62046 (10)	0.6992 (2)	0.29819 (8)	0.0505 (3)
C12	0.63343 (11)	0.6046 (3)	0.22279 (9)	0.0575 (4)
H12A	0.6915	0.5076	0.2353	0.069*
H12B	0.6472	0.7230	0.1901	0.069*
C13	0.54145 (11)	0.4765 (2)	0.17534 (8)	0.0508 (3)
C14	0.51482 (11)	0.3025 (2)	0.22953 (8)	0.0527 (3)
H14A	0.4494	0.2406	0.2030	0.063*
H14B	0.5640	0.1847	0.2371	0.063*
C15	0.56696 (15)	0.3622 (3)	0.10559 (10)	0.0780 (5)
H15A	0.5103	0.2760	0.0771	0.117*
H15B	0.6244	0.2682	0.1251	0.117*
H15C	0.5823	0.4707	0.0707	0.117*
C16	0.45296 (13)	0.6332 (3)	0.14473 (10)	0.0704 (5)
H16A	0.4715	0.7444	0.1124	0.106*
H16B	0.4358	0.7012	0.1889	0.106*
H16C	0.3958	0.5527	0.1137	0.106*
O1	0.65928 (9)	0.87306 (19)	0.32485 (7)	0.0688 (3)
Cl1	0.19413 (4)	−0.47224 (9)	0.52256 (3)	0.08168 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0494 (7)	0.0594 (9)	0.0550 (8)	−0.0006 (7)	0.0112 (6)	0.0115 (7)
C2	0.0715 (10)	0.0726 (11)	0.0450 (8)	−0.0080 (8)	0.0157 (7)	−0.0013 (7)
C3	0.0696 (9)	0.0585 (9)	0.0504 (8)	−0.0135 (7)	0.0139 (7)	−0.0063 (7)
C4	0.0477 (7)	0.0489 (8)	0.0500 (7)	0.0014 (6)	0.0124 (6)	0.0008 (6)
C5	0.0621 (8)	0.0566 (9)	0.0551 (8)	−0.0045 (7)	0.0192 (7)	−0.0078 (7)
C6	0.0598 (8)	0.0542 (9)	0.0627 (9)	−0.0087 (7)	0.0150 (7)	−0.0033 (7)
C7	0.0558 (8)	0.0525 (8)	0.0481 (7)	0.0004 (6)	0.0155 (6)	−0.0010 (6)
C8	0.0572 (8)	0.0558 (8)	0.0468 (7)	−0.0018 (7)	0.0150 (6)	−0.0011 (6)
C9	0.0470 (7)	0.0471 (7)	0.0458 (7)	0.0024 (6)	0.0100 (5)	0.0007 (6)
C10	0.0564 (8)	0.0568 (8)	0.0448 (7)	−0.0035 (7)	0.0126 (6)	−0.0069 (6)
C11	0.0441 (6)	0.0506 (8)	0.0526 (8)	−0.0005 (6)	0.0059 (6)	−0.0008 (6)
C12	0.0507 (8)	0.0647 (9)	0.0602 (9)	−0.0044 (7)	0.0206 (6)	−0.0052 (7)
C13	0.0545 (7)	0.0525 (8)	0.0464 (7)	0.0003 (6)	0.0155 (6)	−0.0027 (6)
C14	0.0625 (8)	0.0456 (7)	0.0499 (8)	−0.0012 (6)	0.0153 (6)	−0.0048 (6)
C15	0.0945 (13)	0.0874 (13)	0.0605 (10)	−0.0114 (10)	0.0356 (9)	−0.0178 (9)
C16	0.0686 (10)	0.0708 (11)	0.0614 (9)	0.0072 (9)	0.0000 (8)	0.0082 (8)
O1	0.0740 (7)	0.0596 (7)	0.0712 (7)	−0.0183 (6)	0.0170 (6)	−0.0110 (5)
Cl1	0.0819 (3)	0.0909 (4)	0.0745 (3)	−0.0193 (2)	0.0250 (2)	0.0201 (2)

Geometric parameters (Å, º)

C1—C6	1.373 (2)	C10—C11	1.457 (2)
C1—C2	1.375 (2)	C10—H10	0.9300
C1—Cl1	1.7356 (15)	C11—O1	1.2192 (17)
C2—C3	1.375 (2)	C11—C12	1.494 (2)
C2—H2	0.9300	C12—C13	1.526 (2)
C3—C4	1.390 (2)	C12—H12A	0.9700
C3—H3	0.9300	C12—H12B	0.9700
C4—C5	1.390 (2)	C13—C16	1.525 (2)
C4—C7	1.463 (2)	C13—C15	1.526 (2)
C5—C6	1.378 (2)	C13—C14	1.531 (2)
C5—H5	0.9300	C14—H14A	0.9700
C6—H6	0.9300	C14—H14B	0.9700
C7—C8	1.327 (2)	C15—H15A	0.9600
C7—H7	0.9300	C15—H15B	0.9600
C8—C9	1.4560 (19)	C15—H15C	0.9600
C8—H8	0.9300	C16—H16A	0.9600
C9—C10	1.342 (2)	C16—H16B	0.9600
C9—C14	1.5006 (19)	C16—H16C	0.9600
C6—C1—C2	121.00 (14)	C10—C11—C12	116.55 (12)
C6—C1—Cl1	119.47 (12)	C11—C12—C13	113.41 (12)
C2—C1—Cl1	119.53 (12)	C11—C12—H12A	108.9
C3—C2—C1	119.04 (14)	C13—C12—H12A	108.9
C3—C2—H2	120.5	C11—C12—H12B	108.9
C1—C2—H2	120.5	C13—C12—H12B	108.9
C2—C3—C4	121.89 (14)	H12A—C12—H12B	107.7
C2—C3—H3	119.1	C16—C13—C15	109.80 (14)
C4—C3—H3	119.1	C16—C13—C12	109.72 (13)
C3—C4—C5	117.22 (13)	C15—C13—C12	109.33 (13)
C3—C4—C7	123.38 (13)	C16—C13—C14	110.34 (13)
C5—C4—C7	119.39 (13)	C15—C13—C14	109.04 (13)
C6—C5—C4	121.67 (14)	C12—C13—C14	108.58 (12)
C6—C5—H5	119.2	C9—C14—C13	114.60 (12)
C4—C5—H5	119.2	C9—C14—H14A	108.6
C1—C6—C5	119.18 (14)	C13—C14—H14A	108.6
C1—C6—H6	120.4	C9—C14—H14B	108.6
C5—C6—H6	120.4	C13—C14—H14B	108.6
C8—C7—C4	126.92 (14)	H14A—C14—H14B	107.6
C8—C7—H7	116.5	C13—C15—H15A	109.5
C4—C7—H7	116.5	C13—C15—H15B	109.5
C7—C8—C9	126.19 (14)	H15A—C15—H15B	109.5
C7—C8—H8	116.9	C13—C15—H15C	109.5
C9—C8—H8	116.9	H15A—C15—H15C	109.5
C10—C9—C8	119.59 (13)	H15B—C15—H15C	109.5
C10—C9—C14	120.39 (13)	C13—C16—H16A	109.5
C8—C9—C14	119.99 (12)	C13—C16—H16B	109.5

C9—C10—C11	123.40 (13)	H16A—C16—H16B	109.5
C9—C10—H10	118.3	C13—C16—H16C	109.5
C11—C10—H10	118.3	H16A—C16—H16C	109.5
O1—C11—C10	121.60 (14)	H16B—C16—H16C	109.5
O1—C11—C12	121.83 (14)		

C6—C1—C2—C3	−0.1 (2)	C8—C9—C10—C11	177.38 (13)
Cl1—C1—C2—C3	−179.65 (12)	C14—C9—C10—C11	−0.7 (2)
C1—C2—C3—C4	0.3 (3)	C9—C10—C11—O1	175.58 (14)
C2—C3—C4—C5	−0.2 (2)	C9—C10—C11—C12	−5.8 (2)
C2—C3—C4—C7	−179.28 (14)	O1—C11—C12—C13	−147.07 (14)
C3—C4—C5—C6	−0.1 (2)	C10—C11—C12—C13	34.32 (19)
C7—C4—C5—C6	179.07 (13)	C11—C12—C13—C16	66.81 (17)
C2—C1—C6—C5	−0.1 (2)	C11—C12—C13—C15	−172.71 (14)
Cl1—C1—C6—C5	179.41 (11)	C11—C12—C13—C14	−53.85 (17)
C4—C5—C6—C1	0.2 (2)	C10—C9—C14—C13	−21.6 (2)
C3—C4—C7—C8	−0.4 (2)	C8—C9—C14—C13	160.34 (12)
C5—C4—C7—C8	−179.51 (14)	C16—C13—C14—C9	−72.87 (16)
C4—C7—C8—C9	178.10 (13)	C15—C13—C14—C9	166.46 (13)
C7—C8—C9—C10	−178.00 (15)	C12—C13—C14—C9	47.41 (16)
C7—C8—C9—C14	0.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.93	2.41	3.301 (2)	159
C14—H14*B*···O1^{ii}	0.97	2.57	3.4299 (18)	148

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