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Bis[5-chloro-2-(prop-2-yn-1-yloxy)-phenyl]methane

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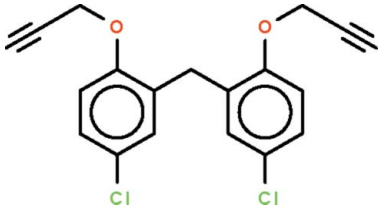
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.099; data-to-parameter ratio = 16.3.

The molecule of the title compound, $C_{19}H_{14}Cl_2O_2$, has two benzene rings connected to a methylene C atom, and the rings are aligned at 66.3 (1)°. Intermolecular C—H$\cdots\pi$ and π–π stacking interactions are observed in the crystal structure, the centroid–centroid distances between parallel benzene rings being 3.7529 (12) and 3.6201 (12) Å, respectively.

Related literature

For a related structure, see: Hussain *et al.* (2009).



Experimental

Crystal data

$C_{19}H_{14}Cl_2O_2$
M_r = 345.20
Triclinic, $P\overline{1}$
a = 8.4844 (5) Å
b = 9.7845 (6) Å
c = 11.2568 (6) Å
α = 86.258 (5)°
β = 71.412 (5)°
γ = 64.707 (6)°
V = 798.08 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.815, T_{max} = 1.000
6118 measured reflections
3523 independent reflections
2975 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.099
S = 1.00
3523 reflections
216 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

Cg is the centroid of the C11–C16 benzene ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C6—H6$\cdots Cg^{i}$	0.95	2.60	3.471 (2)	153

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5147).

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Hussain, Z., Shah, M. R., Anis, I. & Ng, S. W. (2009). *Acta Cryst.* E**65**, o907.
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supporting information

Acta Cryst. (2011). E**67**, o530 [doi:10.1107/S1600536811003205]

Bis[5-chloro-2-(prop-2-yn-1-yloxy)phenyl]methane

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S1. Comment

We have reported several compounds that adopt a V-shape; this shape is induced by a methylene linkage to two aromatic systems. An example is bis[2-(3-bromopropoxy)-5-methylphenyl]methane, which methyl carbon has a widened angle of 115.0 (2)° (Hussain *et al.*, 2009). The methylene angle in the present compound (Scheme I, Fig. 1) is similar [114.4 (1) °]. Two two aromatic rings that are connected the methylene carbon are aligned at 66.3 (1)°. Intermolecular C—H···π interaction occurs between inversion center related molecules (Table 1). π-π stacking is also present between parallel benzene rings in the crystal structure, centroid-to-centroid distances being 3.7529 (12) Å between C1-ring and C1^{i}-ring (symmetry code: (i) 1-x, 1-y, 1-z), and 3.6201 (12) Å between C11-ring and C11^{ii}-ring (symmetry code: (ii) 2-x, 1-y, -z).

S2. Experimental

2, 2′-Methylenebis(4-chlorophenol) (1 g, 3.7 mmol) was dissolved in ethanol (30 ml). Potassium carbonate (1.5 g, 11 mmol) was added and the mixture was heated for an hour. Propargyl bromide (2 ml, 22 mmol) was added and the heating continues for another 3 h. Water (50 ml) was added. The organic compound was extracted by ethyl acetate (50 ml). Slow evaporation of ethyl acetate solution afforded crystals in 80% yield.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 to 0.99 Å, U_{iso}(H) 1.2U_{eq}(C)] and were included in the refinement in the riding model approximation.

The acetylenic H-atoms were located in a difference Fourier map, and were refined with a distance of C–H 0.95±0.01 Å; their temperature factors were refined.

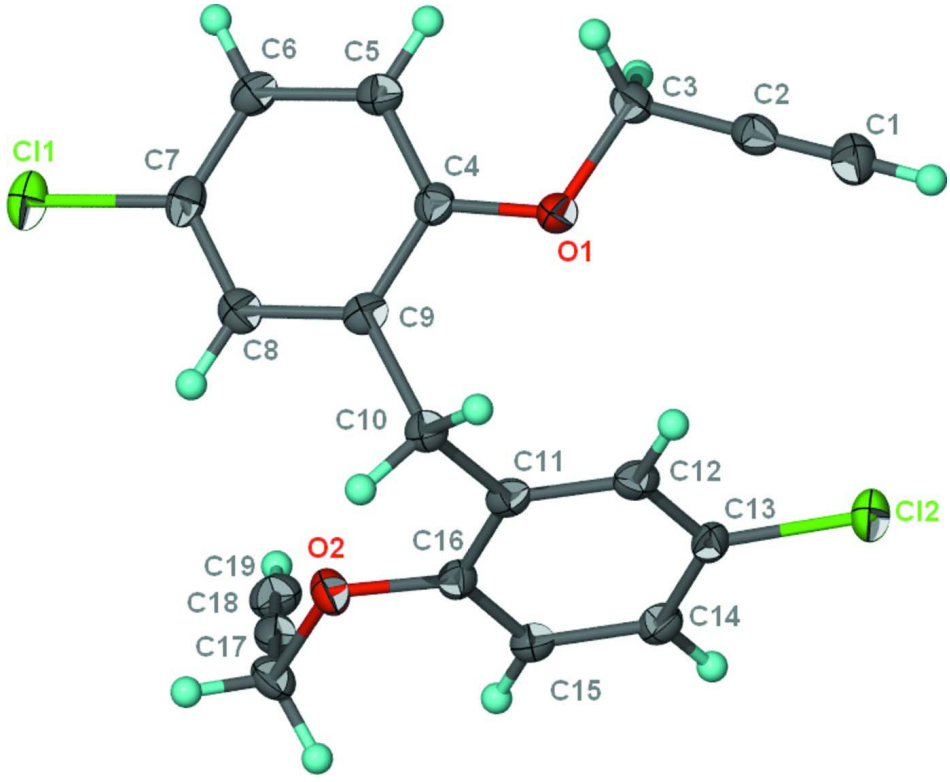

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{19}H_{14}Cl_2O_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Bis[5-chloro-2-(prop-2-yn-1-yloxy)phenyl]methane

Crystal data

$C_{19}H_{14}Cl_2O_2$
M_r = 345.20
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.4844 (5) Å
b = 9.7845 (6) Å
c = 11.2568 (6) Å
α = 86.258 (5)°
β = 71.412 (5)°
γ = 64.707 (6)°
V = 798.08 (8) Å^3
Z = 2
$F(000)$ = 356
D_x = 1.436 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3298 reflections
θ = 2.3–29.2°
μ = 0.41 mm^{-1}
T = 100 K
Prism, colorless
0.30 × 0.25 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.815, T_{max} = 1.000
6118 measured reflections
3523 independent reflections
2975 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −9→10
k = −10→12
l = −11→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.099$
$S = 1.00$
3523 reflections
216 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.2682P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.85099 (6)	0.23350 (5)	0.67998 (4)	0.02285 (13)
Cl2	0.50877 (6)	0.78470 (5)	−0.01311 (4)	0.02450 (13)
O1	0.55177 (16)	0.77464 (14)	0.41682 (11)	0.0196 (3)
O2	1.00711 (16)	0.26968 (13)	0.18471 (11)	0.0182 (3)
C1	0.3290 (3)	1.1163 (2)	0.32429 (18)	0.0228 (4)
C2	0.3478 (2)	1.0165 (2)	0.39167 (16)	0.0182 (4)
C3	0.3745 (2)	0.89566 (19)	0.47714 (16)	0.0175 (4)
H3A	0.3701	0.9327	0.5584	0.021*
H3B	0.2769	0.8603	0.4932	0.021*
C4	0.6114 (2)	0.65014 (19)	0.48288 (15)	0.0158 (4)
C5	0.5100 (2)	0.6355 (2)	0.60376 (16)	0.0176 (4)
H5	0.3909	0.7132	0.6444	0.021*
C6	0.5838 (2)	0.5070 (2)	0.66444 (16)	0.0176 (4)
H6	0.5161	0.4960	0.7469	0.021*
C7	0.7568 (2)	0.3954 (2)	0.60351 (16)	0.0176 (4)
C8	0.8582 (2)	0.4087 (2)	0.48282 (16)	0.0172 (4)
H8	0.9766	0.3300	0.4425	0.021*
C9	0.7868 (2)	0.5366 (2)	0.42099 (15)	0.0154 (3)
C10	0.8966 (2)	0.5563 (2)	0.29023 (15)	0.0161 (4)
H10A	0.8890	0.6602	0.2891	0.019*
H10B	1.0276	0.4843	0.2730	0.019*
C11	0.8327 (2)	0.5312 (2)	0.18567 (15)	0.0151 (3)
C12	0.7154 (2)	0.6527 (2)	0.13844 (16)	0.0170 (4)
H12	0.6728	0.7530	0.1729	0.020*
C13	0.6599 (2)	0.6288 (2)	0.04161 (16)	0.0172 (4)
C14	0.7199 (2)	0.4852 (2)	−0.01130 (16)	0.0178 (4)
H14	0.6819	0.4705	−0.0783	0.021*
C15	0.8372 (2)	0.3614 (2)	0.03478 (16)	0.0167 (4)
H15	0.8794	0.2615	−0.0005	0.020*
C16	0.8922 (2)	0.38484 (19)	0.13286 (15)	0.0155 (3)
C17	1.0784 (2)	0.1178 (2)	0.13135 (17)	0.0199 (4)
H17A	1.1792	0.0504	0.1634	0.024*
H17B	1.1309	0.1149	0.0389	0.024*

C18	0.9368 (2)	0.0606 (2)	0.16123 (16)	0.0196 (4)
C19	0.8221 (3)	0.0152 (2)	0.18736 (17)	0.0232 (4)
H1	0.317 (3)	1.1950 (19)	0.2701 (17)	0.033 (6)*
H19	0.729 (2)	−0.020 (3)	0.209 (2)	0.039 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0291 (3)	0.0206 (2)	0.0249 (2)	−0.0126 (2)	−0.01521 (19)	0.00937 (18)
Cl2	0.0240 (2)	0.0226 (3)	0.0224 (2)	−0.0051 (2)	−0.00986 (18)	0.00816 (18)
O1	0.0207 (6)	0.0165 (6)	0.0147 (6)	−0.0038 (5)	−0.0032 (5)	0.0024 (5)
O2	0.0191 (6)	0.0138 (6)	0.0207 (6)	−0.0033 (5)	−0.0100 (5)	−0.0003 (5)
C1	0.0210 (9)	0.0223 (10)	0.0237 (10)	−0.0072 (8)	−0.0089 (7)	0.0042 (8)
C2	0.0143 (8)	0.0201 (9)	0.0187 (9)	−0.0053 (7)	−0.0055 (7)	−0.0031 (7)
C3	0.0150 (8)	0.0176 (9)	0.0174 (9)	−0.0046 (7)	−0.0049 (7)	−0.0006 (7)
C4	0.0191 (9)	0.0154 (8)	0.0145 (8)	−0.0074 (7)	−0.0074 (7)	0.0012 (7)
C5	0.0173 (8)	0.0191 (9)	0.0161 (9)	−0.0080 (7)	−0.0046 (7)	−0.0002 (7)
C6	0.0200 (9)	0.0209 (9)	0.0151 (8)	−0.0120 (8)	−0.0056 (7)	0.0026 (7)
C7	0.0229 (9)	0.0185 (9)	0.0182 (9)	−0.0120 (8)	−0.0115 (7)	0.0052 (7)
C8	0.0166 (8)	0.0175 (9)	0.0194 (9)	−0.0075 (7)	−0.0077 (7)	0.0002 (7)
C9	0.0171 (8)	0.0182 (9)	0.0146 (8)	−0.0103 (7)	−0.0057 (6)	0.0004 (7)
C10	0.0156 (8)	0.0169 (9)	0.0161 (8)	−0.0074 (7)	−0.0049 (6)	0.0011 (7)
C11	0.0137 (8)	0.0191 (9)	0.0138 (8)	−0.0097 (7)	−0.0023 (6)	0.0019 (7)
C12	0.0177 (8)	0.0164 (9)	0.0153 (8)	−0.0091 (7)	−0.0011 (6)	0.0021 (7)
C13	0.0143 (8)	0.0197 (9)	0.0140 (8)	−0.0059 (7)	−0.0029 (6)	0.0061 (7)
C14	0.0155 (8)	0.0246 (10)	0.0141 (8)	−0.0093 (8)	−0.0050 (6)	0.0022 (7)
C15	0.0172 (8)	0.0177 (9)	0.0138 (8)	−0.0072 (7)	−0.0037 (6)	−0.0003 (7)
C16	0.0132 (8)	0.0180 (9)	0.0141 (8)	−0.0065 (7)	−0.0035 (6)	0.0035 (7)
C17	0.0188 (9)	0.0151 (9)	0.0213 (9)	−0.0023 (7)	−0.0068 (7)	−0.0026 (7)
C18	0.0232 (9)	0.0155 (9)	0.0151 (9)	−0.0029 (8)	−0.0070 (7)	−0.0012 (7)
C19	0.0279 (10)	0.0231 (10)	0.0172 (9)	−0.0107 (9)	−0.0056 (7)	−0.0002 (7)

Geometric parameters (Å, º)

Cl1—C7	1.7518 (18)	C8—H8	0.9500
Cl2—C13	1.7492 (18)	C9—C10	1.521 (2)
O1—C4	1.374 (2)	C10—C11	1.516 (2)
O1—C3	1.435 (2)	C10—H10A	0.9900
O2—C16	1.378 (2)	C10—H10B	0.9900
O2—C17	1.432 (2)	C11—C12	1.389 (2)
C1—C2	1.183 (3)	C11—C16	1.400 (2)
C1—H1	0.94 (2)	C12—C13	1.385 (2)
C2—C3	1.462 (2)	C12—H12	0.9500
C3—H3A	0.9900	C13—C14	1.376 (3)
C3—H3B	0.9900	C14—C15	1.394 (2)
C4—C9	1.401 (2)	C14—H14	0.9500
C4—C5	1.395 (2)	C15—C16	1.394 (2)
C5—C6	1.389 (2)	C15—H15	0.9500

C5—H5	0.9500	C17—C18	1.470 (3)
C6—C7	1.379 (3)	C17—H17A	0.9900
C6—H6	0.9500	C17—H17B	0.9900
C7—C8	1.389 (2)	C18—C19	1.184 (3)
C8—C9	1.387 (2)	C19—H19	0.95 (2)

C4—O1—C3	117.28 (13)	C9—C10—H10A	108.7
C16—O2—C17	117.67 (13)	C11—C10—H10B	108.7
C2—C1—H1	178.8 (13)	C9—C10—H10B	108.7
C1—C2—C3	177.80 (19)	H10A—C10—H10B	107.6
O1—C3—C2	106.72 (13)	C12—C11—C16	118.08 (15)
O1—C3—H3A	110.4	C12—C11—C10	121.02 (15)
C2—C3—H3A	110.4	C16—C11—C10	120.89 (15)
O1—C3—H3B	110.4	C13—C12—C11	120.63 (16)
C2—C3—H3B	110.4	C13—C12—H12	119.7
H3A—C3—H3B	108.6	C11—C12—H12	119.7
O1—C4—C9	115.07 (14)	C14—C13—C12	121.33 (16)
O1—C4—C5	123.85 (15)	C14—C13—Cl2	119.55 (14)
C9—C4—C5	121.06 (16)	C12—C13—Cl2	119.12 (14)
C6—C5—C4	119.73 (16)	C13—C14—C15	119.11 (16)
C6—C5—H5	120.1	C13—C14—H14	120.4
C4—C5—H5	120.1	C15—C14—H14	120.4
C7—C6—C5	119.16 (16)	C14—C15—C16	119.73 (16)
C7—C6—H6	120.4	C14—C15—H15	120.1
C5—C6—H6	120.4	C16—C15—H15	120.1
C6—C7—C8	121.46 (16)	O2—C16—C15	123.84 (16)
C6—C7—Cl1	119.33 (13)	O2—C16—C11	115.05 (15)
C8—C7—Cl1	119.21 (14)	C15—C16—C11	121.11 (16)
C9—C8—C7	120.16 (16)	O2—C17—C18	112.48 (14)
C9—C8—H8	119.9	O2—C17—H17A	109.1
C7—C8—H8	119.9	C18—C17—H17A	109.1
C8—C9—C4	118.44 (15)	O2—C17—H17B	109.1
C8—C9—C10	121.38 (15)	C18—C17—H17B	109.1
C4—C9—C10	120.17 (15)	H17A—C17—H17B	107.8
C11—C10—C9	114.36 (13)	C19—C18—C17	178.90 (19)
C11—C10—H10A	108.7	C18—C19—H19	179.4 (15)

C4—O1—C3—C2	176.88 (13)	C9—C10—C11—C12	97.47 (18)
C3—O1—C4—C9	−178.72 (14)	C9—C10—C11—C16	−83.30 (19)
C3—O1—C4—C5	0.0 (2)	C16—C11—C12—C13	−0.2 (2)
O1—C4—C5—C6	−178.32 (15)	C10—C11—C12—C13	179.03 (15)
C9—C4—C5—C6	0.3 (3)	C11—C12—C13—C14	−0.5 (2)
C4—C5—C6—C7	−0.2 (3)	C11—C12—C13—Cl2	178.86 (12)
C5—C6—C7—C8	−0.2 (3)	C12—C13—C14—C15	0.8 (2)
C5—C6—C7—Cl1	179.66 (13)	Cl2—C13—C14—C15	−178.63 (13)
C6—C7—C8—C9	0.5 (3)	C13—C14—C15—C16	−0.2 (2)
Cl1—C7—C8—C9	−179.40 (12)	C17—O2—C16—C15	2.2 (2)
C7—C8—C9—C4	−0.3 (2)	C17—O2—C16—C11	−177.57 (14)

C7—C8—C9—C10	178.34 (15)	C14—C15—C16—O2	179.79 (15)
O1—C4—C9—C8	178.68 (14)	C14—C15—C16—C11	−0.5 (2)
C5—C4—C9—C8	−0.1 (2)	C12—C11—C16—O2	−179.54 (14)
O1—C4—C9—C10	0.0 (2)	C10—C11—C16—O2	1.2 (2)
C5—C4—C9—C10	−178.76 (15)	C12—C11—C16—C15	0.7 (2)
C8—C9—C10—C11	105.02 (18)	C10—C11—C16—C15	−178.53 (15)
C4—C9—C10—C11	−76.4 (2)	C16—O2—C17—C18	−71.59 (19)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C11–C16 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···*Cg*^{i}	0.95	2.60	3.471 (2)	153

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