Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (*E*,*E*,*E*)-1,6-Bis(4-chlorophenyl)hexa-1,3,5-triene

**Zhiying Li**

Departmemt of Chemistry, Xinzhou Teachers University, Xinzhou, Shanxi 030006, People's Republic of China
Correspondence e-mail: liubin@sxu.edu.cn

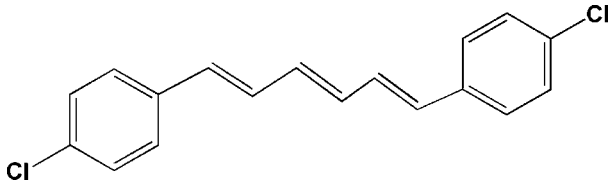
Received 2 April 2013; accepted 6 April 2013

Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.039; $wR$ factor = 0.105; data-to-parameter ratio = 17.1.

The title molecule, $C_{18}H_{14}Cl_2$, lies about an inversion centre. The hexatriene chain is planar with a maximum deviation of 0.0001 (17) Å. The torsion angle of the single bond between the chain and the benzene ring is −168.49 (17)°. In the crystal, the shortest intermolecular distance between the Cl atoms is 4.0785 (11) Å.

## Related literature

For the preparation, see: Spangler *et al.* (1989). For luminescence and fluorescent properties of *trans*-diphenyl polyenes, see: Alford & Palmer (1986); Sonoda *et al.*(2003).




## Experimental

### *Crystal data*

$C_{18}H_{14}Cl_2$ $M_r$ = 301.19
Monoclinic, $P2_1/c$
$a$ = 15.6277 (7) Å
$b$ = 4.0784 (2) Å
$c$ = 12.1026 (5) Å
$\beta$ = 105.810 (4)°
$V$ = 742.20 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.42 mm$^{-1}$
$T$ = 291 K
0.42 × 0.38 × 0.30 mm

### *Data collection*

Agilent SuperNova (Dual, Cu at zero, Eos) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.667, $T_{max}$ = 1.000
2513 measured reflections
1560 independent reflections
1214 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.013

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
$S$ = 1.06
1560 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *OLEX2* (Dolomanov *et al.*, 2009) and *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2*; software used to prepare material for publication: *OLEX2*.

We acknowledge the Scientific and Technological Development Project funding of colleges and universities in Shanxi Province (20111023)

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2085).

## References

Agilent (2012). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, England.
Alford, P. C. & Palmer, T. F. (1986). *Chem. Phys. Lett.* **127**, 19–25.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sonoda, Y., Kawanishi, Y. & Goto, M. (2003). *Acta Cryst.* C**59**, o311–o313.
Spangler, C. W., McCoy, R. K., Dembek, A. A., Sapochak, L. S. & Gates, B. D. (1989). *J. Chem. Soc. Perkin Trans 1*, pp. 151–154.

# supporting information

*Acta Cryst.* (2013). E**69**, o699 [https://doi.org/10.1107/S160053681300932X]

## (*E*,*E*,*E*)-1,6-Bis(4-chlorophenyl)hexa-1,3,5-triene

**Zhiying Li**

### S1. Comment

The luminescence properties of the linear all-*trans*-diphenyl polyenes Ph-(CH=CH)$_n$—Ph (DPH) have been the subject of numerous investigations(Sonoda *et al.*(2003)). The emission properties of DPH and its derivatives in solution have been extensively studied because of its unique fluorescence behavior(Alford & Palmer,1986). DPH is known to exhibit dual fluorescence from $S_1$ and $S_2$ at thermal equilibrium. The crystal structure of (*E*,*E*,*E*)-1,6-bis(2,4-dichlorophenyl)-hexa-1,3,5-triene has been studied (Sonoda *et al.*2003). In the crystal structure of the related compound, *E*,*E*,*E*-1,6-bis(*p*-chlorophenyl)- 1,3,5-hexatriene, the benzene rings are $\pi\cdots\pi$ stacked with unit translation along the *b*-axis with a centroid to centroid distance of 4.0785 (11)Å, a perpendicular distance between the planes of 3.4728 (8)Å and a slippage of 2.139Å.

### S2. Experimental

The compound was prepared and purified as described previously (Spangler *et al.*1989). Crystals suitable for the X-ray diffraction study was obtained free evaporation of an solvent chloroform from a highly diluted solution in the dark at room temperature.

### S3. Refinement

H atoms attached to C atoms were placed in geometrically idealized positions with C$sp^2$ = 0.930 Å,and constrained to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$.

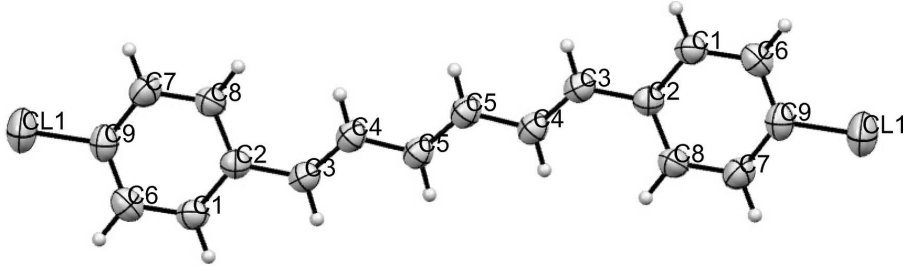



**Figure 1**

The structure of the title compound in 30% probability ellipsoids. H atoms are shown as small spheres of arbitrary radii.

### *trans*,*trans*,*trans*-1,6-Bis(4-chlorophenyl)hexa-1,3,5-triene

*Crystal data*

| | |
|---|---|
| $C_{18}H_{14}Cl_2$ | $a$ = 15.6277 (7) Å |
| $M_r$ = 301.19 | $b$ = 4.0784 (2) Å |
| Monoclinic, $P2_1/c$ | $c$ = 12.1026 (5) Å |
| Hall symbol: -P 2ybc | $\beta$ = 105.810 (4)° |

$V$ = 742.20 (5) Å$^3$
$Z$ = 2
$F$(000) = 312
$D_x$ = 1.348 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.7107 Å
Cell parameters from 971 reflections

$\theta$ = 3.4–28.6°
$\mu$ = 0.42 mm$^{-1}$
$T$ = 291 K
Block, yellow
0.42 × 0.38 × 0.30 mm

*Data collection*

Agilent SuperNova (Dual, Cu at zero, Eos) diffractometer
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 16.0733 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)

$T_{min}$ = 0.667, $T_{max}$ = 1.000
2513 measured reflections
1560 independent reflections
1214 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.013
$\theta_{max}$ = 26.7°, $\theta_{min}$ = 3.4°
$h$ = −11→19
$k$ = −4→5
$l$ = −15→15

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
$S$ = 1.06
1560 reflections
91 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
$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.1061P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

*Special details*

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

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.94481 (3) | 0.31466 (16) | 0.62511 (5) | 0.0747 (3) |
| C1 | 0.70850 (12) | 0.6448 (4) | 0.44590 (15) | 0.0465 (4) |
| H1 | 0.6623 | 0.7651 | 0.4608 | 0.056* |
| C2 | 0.70013 (10) | 0.5327 (4) | 0.33486 (14) | 0.0396 (4) |
| C3 | 0.61893 (11) | 0.6044 (4) | 0.24400 (15) | 0.0440 (4) |
| H3 | 0.5806 | 0.7576 | 0.2617 | 0.053* |
| C4 | 0.59348 (11) | 0.4758 (4) | 0.13885 (14) | 0.0428 (4) |
| H4 | 0.6301 | 0.3187 | 0.1196 | 0.051* |
| C5 | 0.51318 (11) | 0.5638 (4) | 0.05308 (14) | 0.0442 (4) |
| H5 | 0.4768 | 0.7210 | 0.0727 | 0.053* |
| C6 | 0.78361 (12) | 0.5819 (4) | 0.53446 (15) | 0.0491 (5) |
| H6 | 0.7879 | 0.6593 | 0.6081 | 0.059* |
| C7 | 0.84667 (12) | 0.2943 (5) | 0.40343 (16) | 0.0512 (5) |
| H7 | 0.8936 | 0.1769 | 0.3892 | 0.061* |

| | | | | |
|---|---|---|---|---|
| C8 | 0.77155 (11) | 0.3594 (4) | 0.31545 (15) | 0.0462 (4) |
| H8 | 0.7685 | 0.2863 | 0.2417 | 0.055* |
| C9 | 0.85169 (11) | 0.4047 (4) | 0.51293 (15) | 0.0473 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0578 (3) | 0.0907 (5) | 0.0617 (4) | 0.0025 (3) | −0.0072 (2) | 0.0067 (3) |
| C1 | 0.0474 (10) | 0.0494 (10) | 0.0469 (10) | 0.0036 (8) | 0.0197 (8) | −0.0014 (9) |
| C2 | 0.0397 (8) | 0.0400 (9) | 0.0410 (9) | −0.0025 (7) | 0.0141 (7) | 0.0023 (8) |
| C3 | 0.0416 (9) | 0.0438 (10) | 0.0492 (10) | 0.0039 (7) | 0.0166 (8) | 0.0027 (8) |
| C4 | 0.0401 (8) | 0.0418 (9) | 0.0475 (10) | 0.0008 (7) | 0.0137 (7) | 0.0052 (8) |
| C5 | 0.0399 (9) | 0.0445 (10) | 0.0492 (9) | 0.0010 (7) | 0.0135 (7) | 0.0071 (8) |
| C6 | 0.0569 (11) | 0.0522 (11) | 0.0392 (9) | −0.0052 (9) | 0.0145 (8) | −0.0021 (8) |
| C7 | 0.0406 (9) | 0.0593 (12) | 0.0542 (11) | 0.0056 (8) | 0.0137 (8) | 0.0018 (10) |
| C8 | 0.0458 (9) | 0.0535 (11) | 0.0408 (9) | 0.0003 (8) | 0.0144 (7) | −0.0047 (8) |
| C9 | 0.0432 (9) | 0.0486 (10) | 0.0462 (10) | −0.0058 (8) | 0.0054 (7) | 0.0060 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C9 | 1.7376 (17) | C4—H4 | 0.9300 |
| C1—C6 | 1.381 (2) | C5—C5$^{i}$ | 1.342 (3) |
| C1—C2 | 1.392 (2) | C5—H5 | 0.9300 |
| C1—H1 | 0.9300 | C6—C9 | 1.369 (2) |
| C2—C8 | 1.394 (2) | C6—H6 | 0.9300 |
| C2—C3 | 1.464 (2) | C7—C8 | 1.379 (2) |
| C3—C4 | 1.333 (2) | C7—C9 | 1.382 (3) |
| C3—H3 | 0.9300 | C7—H7 | 0.9300 |
| C4—C5 | 1.439 (2) | C8—H8 | 0.9300 |
| | | | |
| C6—C1—C2 | 121.66 (16) | C4—C5—H5 | 117.5 |
| C6—C1—H1 | 119.2 | C9—C6—C1 | 119.39 (17) |
| C2—C1—H1 | 119.2 | C9—C6—H6 | 120.3 |
| C1—C2—C8 | 117.41 (15) | C1—C6—H6 | 120.3 |
| C1—C2—C3 | 119.58 (15) | C8—C7—C9 | 119.45 (17) |
| C8—C2—C3 | 122.99 (15) | C8—C7—H7 | 120.3 |
| C4—C3—C2 | 127.62 (16) | C9—C7—H7 | 120.3 |
| C4—C3—H3 | 116.2 | C7—C8—C2 | 121.33 (17) |
| C2—C3—H3 | 116.2 | C7—C8—H8 | 119.3 |
| C3—C4—C5 | 124.43 (17) | C2—C8—H8 | 119.3 |
| C3—C4—H4 | 117.8 | C6—C9—C7 | 120.72 (17) |
| C5—C4—H4 | 117.8 | C6—C9—Cl1 | 119.46 (15) |
| C5$^{i}$—C5—C4 | 125.0 (2) | C7—C9—Cl1 | 119.81 (14) |
| C5$^{i}$—C5—H5 | 117.5 | | |
| | | | |
| C6—C1—C2—C8 | −1.4 (3) | C9—C7—C8—C2 | −0.5 (3) |
| C6—C1—C2—C3 | 179.69 (16) | C1—C2—C8—C7 | 1.6 (3) |
| C1—C2—C3—C4 | −168.49 (17) | C3—C2—C8—C7 | −179.46 (16) |

| | | | |
|---|---|---|---|
| C8—C2—C3—C4 | 12.6 (3) | C1—C6—C9—C7 | 1.3 (3) |
| C2—C3—C4—C5 | −178.71 (16) | C1—C6—C9—Cl1 | −178.05 (13) |
| C3—C4—C5—C5$^{i}$ | 180.0 (2) | C8—C7—C9—C6 | −1.0 (3) |
| C2—C1—C6—C9 | −0.1 (3) | C8—C7—C9—Cl1 | 178.31 (14) |

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