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## 1,8-Dichloro-9,10-dihydro-9,10-ethenoanthracene

MARIA DEL ROSARIO BENITES, ANDREW W. MAVERICK  
AND FRANK R. FRONCZEK

*Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803-1804, USA. E-mail: fronz@chxray1.chem.lsu.edu*

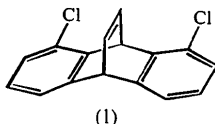
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### Abstract

The title compound, C<sub>16</sub>H<sub>10</sub>Cl<sub>2</sub>, presents a C=C bridge bond length of 1.312(3) Å and C—Cl distances of 1.741(2) and 1.744(2) Å. The dihedral angles between the aromatic rings and the plane formed by the ethene and the bridgehead C atoms are 121.79(8) and 120.76(6)°, and the two phenyl ring planes form a dihedral angle of 117.42(7)°.

### Comment

We have been studying the activation of 1,8-dichloroanthracene derivatives towards nucleophilic substitution via  $\pi$  complexation to CpFe<sup>+</sup> moieties (Cp = cyclopentadienyl) (Benites, Fronczek & Maverick, 1996). We found that  $\pi$  complexation was accompanied by reduction of the 1,8-dichloroanthracene moiety to 1,8-dichloro-9,10-dihydroanthracene. We were interested in the title compound, (1), because its central ring should no longer be subject to reduction.



The bond length of the C=C bridge in compound (1) agrees well with the value of 1.316(3) Å reported for the equivalent C=C double bond in the par-

ent dibenzobarrelene (Trotter & Wireko, 1990) and is somewhat shorter than that in the 15,16-dicarbonyl nitrile derivative [1.343(5) Å; Oliver, Fallon & Smith, 1986] and that in dimethyl 9,10-dimethyl-9,10-dihydro-9,10-ethenoanthracene-11,12-dicarboxylate [1.335(2) Å; Pokkuluri, Scheffer & Trotter, 1993]. The C—Cl distances in (1) [1.741(2) and 1.744(2) Å] are comparable to those in 1,8-dichloroanthracene [1.745(4) and 1.756(4) Å; Benites, Maverick & Fronczek, 1996], 1,8-dichloro-10-methylantracene [1.749 Å; Desvergne, Gaultier & Hauw, 1970] and 1,8-dichloro-9-methylantracene [1.726(7) Å; Dellaca, Penfold & Robinson, 1969]. The maximum deviation of the aromatic rings of (1) from planarity is 0.010(2) Å (for C11). The Cl atoms lie slightly out of these planes, with deviations of 0.0281(6) Å for Cl1 and 0.0166(5) Å for Cl2. The C1—C11—C12 and C8—C13—C14 angles are smaller by an average of 2.3(2)° than C4—C12—C11 and C5—C14—C13, as a result of the Cl substitution. The structure of the molecule analogous to the title compound with methoxycarbonyl groups at C15 and C16 has been reported recently (Rettig, Scheffer, Trotter & Yang, 1995), and exhibits the same asymmetry, with a 2.6(2)° difference. This asymmetry is not present in the parent dibenzobarrelene (Trotter & Wireko, 1990). The benzene rings and the plane constituted by the ethene and the bridgehead C atoms (C9 and C10) of the title compound form dihedral angles of 120.76(6) and 121.79(8)°, whereas the aromatic rings make a dihedral angle of 117.42(7)°.

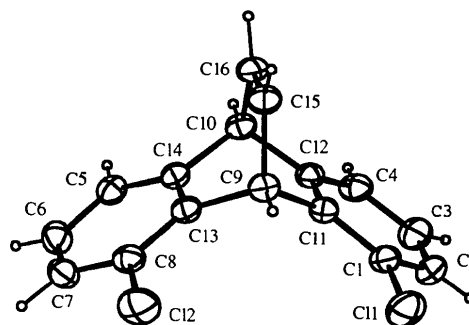


Fig. 1. Molecular structure showing 40% probability ellipsoids. H atoms are illustrated by circles of arbitrary radii.

### Experimental

The compound was synthesized by the Diels–Alder addition reaction [based on the general procedure of Paquette, Moerck, Harirchian & Magnus (1978)] of 1,8-dichloroanthracene with the acetylene synthon phenyl vinyl sulfoxide in chlorobenzene for 8 d (30% isolated yield), and crystallized from CCl<sub>4</sub>–CH<sub>2</sub>Cl<sub>2</sub> by slow evaporation.

**Crystal data**

C<sub>16</sub>H<sub>10</sub>Cl<sub>2</sub>  
*M<sub>r</sub>* = 273.16  
 Monoclinic  
*P*2<sub>1</sub>/*c*  
*a* = 11.217 (1) Å  
*b* = 8.1008 (3) Å  
*c* = 14.4403 (8) Å  
 $\beta$  = 104.34 (1)°  
*V* = 1271.3 (3) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.427 Mg m<sup>-3</sup>  
*D<sub>m</sub>* not measured

**Data collection**

Enraf–Nonius CAD-4  
 diffractometer  
 $\theta/2\theta$  scans  
 Absorption correction:  
 $\psi$  scan (North, Phillips  
 & Mathews, 1968)  
*T<sub>min</sub>* = 0.36, *T<sub>max</sub>* = 0.47  
 2841 measured reflections  
 2532 independent reflections

**Refinement**

Refinement on *F*<sup>2</sup>  
*R* = 0.039  
*wR* = 0.059  
*S* = 2.301  
 2326 reflections  
 204 parameters  
 All H atoms refined  
 $w = 4F_o^2/[\sigma^2(F_o^2) + 0.0009F_o^4]$   
 $(\Delta/\sigma)_{\max} = 0.023$

Cu *K*α radiation  
 $\lambda = 1.54184$  Å  
 Cell parameters from 25  
 reflections  
 $\theta = 19\text{--}29^\circ$   
 $\mu = 4.47$  mm<sup>-1</sup>  
*T* = 297 K  
 Prism  
 0.30 × 0.22 × 0.17 mm  
 Colorless

2326 reflections with  
 $I > \sigma(I)$   
*R<sub>int</sub>* = 0.012  
 $\theta_{\max} = 75^\circ$   
 $h = 0 \rightarrow 14$   
 $k = 0 \rightarrow 9$   
 $l = -18 \rightarrow 17$   
 3 standard reflections  
 frequency: 120 min  
 intensity decay: 3.6%

$\Delta\rho_{\max} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.14$  e Å<sup>-3</sup>  
 Extinction correction:  
 isotropic (Zachariasen,  
 1963)  
 Extinction coefficient:  
 $3.9(2) \times 10^{-6}$   
 Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. Selected geometric parameters (Å, °)

C11—C1	1.741 (2)	C10—C14	1.520 (3)
C12—C8	1.744 (2)	C10—C16	1.529 (2)
C9—C11	1.528 (2)	C11—C12	1.397 (2)
C9—C13	1.520 (3)	C13—C14	1.399 (2)
C9—C15	1.528 (2)	C15—C16	1.312 (3)
C10—C12	1.521 (2)		
C11—C9—C13	104.5 (1)	C10—C12—C11	112.5 (1)
C11—C9—C15	105.8 (1)	C8—C13—C9	128.4 (2)
C13—C9—C15	105.6 (1)	C8—C13—C14	118.7 (2)
C12—C10—C14	105.4 (1)	C9—C13—C14	112.9 (2)
C14—C10—C16	106.0 (1)	C5—C14—C10	126.7 (2)
C1—C11—C9	128.5 (2)	C5—C14—C13	120.9 (2)
C1—C11—C12	118.7 (2)	C10—C14—C13	112.5 (2)
C9—C11—C12	112.8 (1)	C9—C15—C16	114.7 (2)
C4—C12—C10	126.5 (2)	C10—C16—C15	113.9 (1)
C4—C12—C11	121.1 (1)		

C—H distances are in the range 0.86 (2)–0.99 (2) Å, while *B<sub>iso</sub>* values for H atoms are in the range 3.3 (4)–7.1 (7) Å<sup>2</sup>.

Data collection: *CAD-4 Operations Manual* (Enraf–Nonius, 1977). Cell refinement: *CAD-4 Operations Manual*. Data reduction: *PROCESS* in *MolEN* (Fair, 1990). Program(s) used to solve structure: *MULTAN80* (Main *et al.*, 1980). Program(s) used to refine structure: *LSFM* in *MolEN*. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *CIFIN* in *MolEN*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BK1334). Services for accessing these data are described at the back of the journal.

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**1,1,1,4,4,4-Hexachloro-1,4-disilabutane**

NORBERT W. MITZEL, JÜRGEN RIEDE AND HUBERT SCHMIDBAUR

*Anorganisch-Chemisches Institut, Technische Universität München, Lichtenbergstrasse 4, D-85747 Garching, Germany. E-mail: n.w.mitzel@lrz.tu-muenchen.de*

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**Abstract**

Molecules of the title compound, C<sub>2</sub>H<sub>4</sub>Cl<sub>6</sub>Si<sub>2</sub>, have a crystallographic centre of inversion and adopt a *trans* conformation in the crystal. Important bond lengths