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## Key indicators

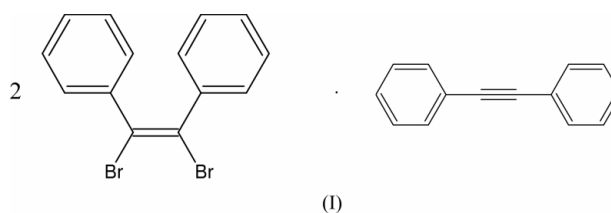
Single-crystal X-ray study  
 $T = 150\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$   
 $R$  factor = 0.055  
 $wR$  factor = 0.148  
Data-to-parameter ratio = 17.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*cis*-1,2-Dibromo-1,2-diphenylethene–  
diphenylethyne (2/1)

The molecular components,  $2\text{C}_{14}\text{H}_{10}\text{Br}_2 \cdot \text{C}_{14}\text{H}_{10}$ , are arranged in separate stacks in this ordered structure. There is no evidence of  $\pi$ – $\pi$  intermolecular interaction. Diphenylethyne lies on a crystallographic inversion centre. The structure can be represented as centrosymmetric trimolecular units, held together by a  $\text{C}-\text{H} \cdots \text{ring}$  interaction between a stilbene and each of the phenyl groups of the diphenylethyne ( $\text{H} \cdots \text{C}_{g_{\text{ring}}}$  2.66 Å;  $\text{C}_{g_{\text{ring}}}$  indicates a ring centroid).

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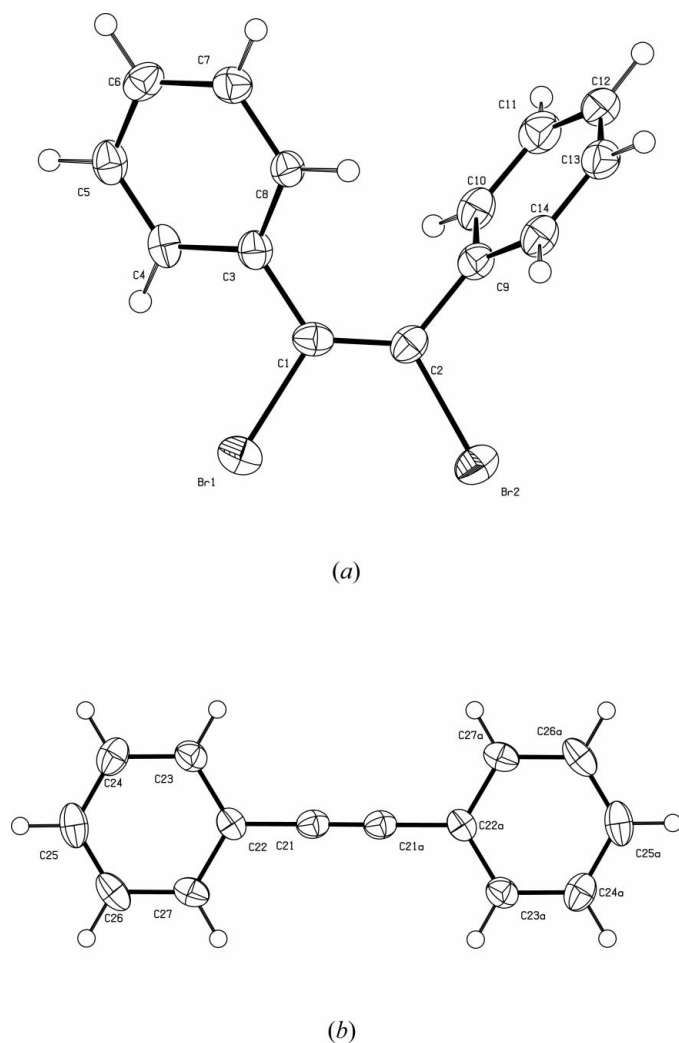
## Comment

*cis*-Stilbene is liquid at room temperature (m.p. 278 K). Crystal structures are known for *cis*-1,2-dichlorostilbene (Hey *et al.*, 1984) and the chloro-substituted stilbene *cis*-bis(4-chlorophenyl)-1,2-dichloroethene (Norrestam *et al.*, 1977).



A sample of *cis*-1,2-dibromostilbene (Chudek & Foster, 2002) had been kept in the dark for at least 30 years. On examination, it was found that the originally dry colourless crystals had become new crystals, up to 2 mm, in a brown bromine-containing liquid. NMR spectra showed that the crystals contained *cis*-1,2-dibromostilbene along with another aromatic component. The structure of this molecular complex, *i.e.* *cis*-1,2-dibromo-1,2-diphenylethene–diphenylethyne (2/1), (I), is reported here.

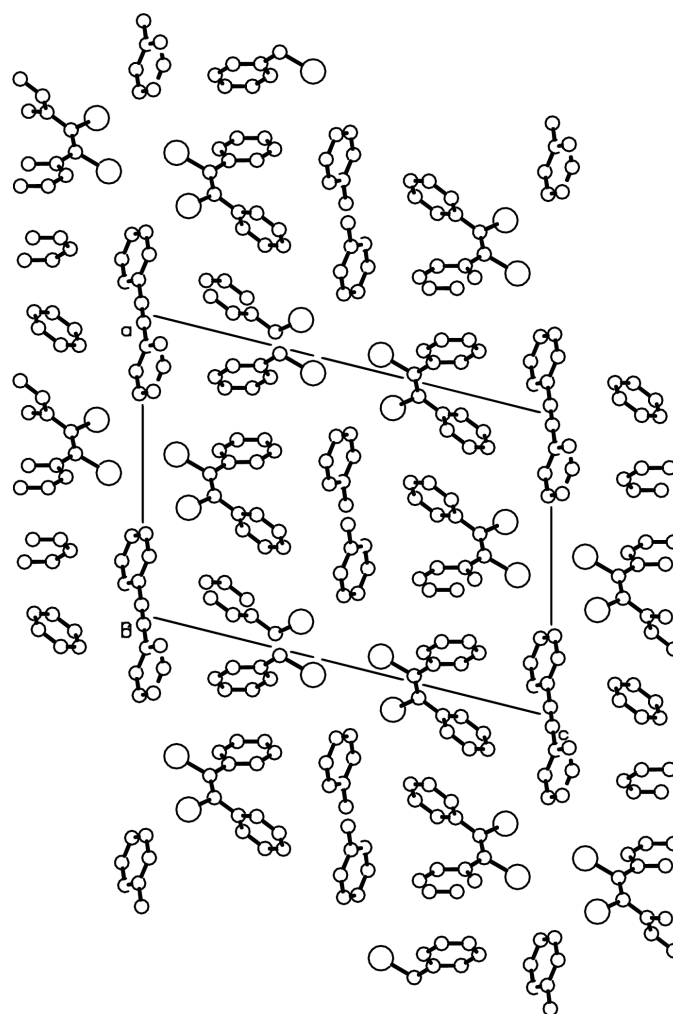
Structure determination showed that the crystals contain an ordered (2:1) assembly of *cis*-1,2-dibromostilbene (1) and diphenylacetylene (2) (Figs. 1 and 2). The stoichiometry is fixed, unlike the solid solutions formed by *trans*-stilbene with *trans*-azobenzene (Bouwstra *et al.*, 1985). Molecules (1) and (2) are arranged in planes parallel to  $ab$ , with (1) at  $z = 0.25$  and (2) at  $z = 0$ . There are separate stacks of (1) and (2) parallel to the  $b$  axis. There is no evidence of  $\pi$ – $\pi$  interaction in these stacks; projections normal to the planes of the phenyl rings show zero overlap with adjacent molecules and the minimum distance between the centres of gravity of parallel rings down the stack is 4.6 Å. There do not appear to be any reports of solid  $\pi$ -complexes of *cis*-stilbenes (Chudek & Foster, 2002), although *trans*-stilbene forms a classical 1:1  $\pi$ -complex with 1,3,5-trinitrobenzene (Bar & Bernstein, 1978) and diphenylacetylene complexes with 1,2,4,5-tetracyanobenzene (Pasiamente *et al.*, 1984).



**Figure 1**  
The structures of (a) *cis*-1,2-dibromodiphenylethene and (b) diphenylacetylene, showing 50% probability displacement ellipsoids

The only significant intermolecular interaction in the present structure is between C7 of the stilbene and the phenyl group of the acetylene ( $\text{H} \cdots \text{Cg}_{\text{ring}}$  2.66 Å;  $\text{Cg}_{\text{ring}}$  indicates a ring centroid) to form isolated centrosymmetric trimolecular units (Fig. 2).

The torsion angles (Table 1) show that molecule (1) is far from symmetrical; the two phenyl rings are arranged very differently. A similar relationship is found in *cis*-1,2-dichlorostilbene but not in *cis*-bis(4-chlorophenyl)-1,2-dichloroethene. In (I), this layout optimizes the contact to the acetylene, but there are no short intermolecular ring–ring or C–H $\cdots$ ring contacts in *cis*-1,2-dichlorostilbene. A simple molecular-mechanics calculation (Advanced Chemical Developments, 2000) predicts a small difference, at most, between the phenyl group torsion angles in each of the isolated molecules. This calculation predicts that the C3–C1–C2–C9 group would be planar. Experimentally, in (1), C3 and C9 are 0.078 (6) and –0.061 (6) Å out of the mean plane Br1–C1–C2–Br2. Table 1 shows that this twist is



**Figure 2**  
Packing diagram, viewed down *b*, showing the trimolecular units.

more marked in both *cis*-1,2-dichlorostilbene and *cis*-bis(4-chloro-phenyl)-1,2-dichloroethene.

Debromination of *trans*-1,2-dibromostilbene derivatives is the traditional route to diphenylacetylenes (e.g. Karrer, 1947). Presumably a similar reaction has occurred spontaneously with the less stable *cis* isomer, but has not gone to completion because of the lattice stabilization of the title complex.

## Experimental

The original *cis*-1,2-dibromostilbene was prepared by a student of R. Foster, *ca* 1965. The sample was stored in glass in the dark for approximately 30 years. No details of the original preparation are available.

### Crystal data

$2\text{C}_{14}\text{H}_{10}\text{Br}_2 \cdot \text{C}_{14}\text{H}_{10}$   
 $M_r = 854.30$   
 Monoclinic,  $P2_1/n$   
 $a = 14.8445$  (5) Å  
 $b = 5.7702$  (3) Å  
 $c = 20.741$  (9) Å  
 $\beta = 104.037$  (2)°  
 $V = 1723.5$  (8) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.646$  Mg m<sup>–3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 13506 reflections  
 $\theta = 1.0$ – $27.1^\circ$   
 $\mu = 4.70$  mm<sup>–1</sup>  
 $T = 150$  (2) K  
 Block, colourless  
 $0.30 \times 0.20 \times 0.15$  mm

## Data collection

Enraf–Nonius KappaCCD area-detector diffractometer	3718 independent reflections
$\varphi$ and $\omega$ scans	2614 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SORTAV; Blessing, 1995)	$R_{\text{int}} = 0.103$
$T_{\text{min}} = 0.946$ , $T_{\text{max}} = 0.999$	$\theta_{\text{max}} = 27.1^\circ$
11791 measured reflections	$h = -19 \rightarrow 18$
	$k = -6 \rightarrow 7$
	$l = -23 \rightarrow 26$

## Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.055$	$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2]$
$wR(F^2) = 0.148$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{\text{max}} = 0.002$
3718 reflections	$\Delta\rho_{\text{max}} = 0.76 \text{ e } \text{\AA}^{-3}$
208 parameters	$\Delta\rho_{\text{min}} = -0.95 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Br1–C1	1.907 (4)	C1–C3	1.474 (6)
Br2–C2	1.912 (4)	C21–C21 <sup>i</sup>	1.188 (9)
C1–C2	1.334 (6)		
C2–C1–C3	126.1 (4)	C1–C2–Br2	122.0 (3)
C2–C1–Br1	119.2 (3)	C9–C2–Br2	112.1 (3)
C3–C1–Br1	114.7 (3)	C21 <sup>i</sup> –C21–C22	178.8 (6)
C1–C2–C9	125.9 (4)		
C4–C3–C1–C2	144.5 (5)	C10–C9–C2–Br2	111.1 (4)
C3–C1–C2–C9	–4.2 (7)	C14–C9–C2–C1	112.5 (5)
C1–C2–C9–C10	–68.6 (6)	Br1–C1–C2–Br2	–2.0 (5)
C4–C3–C1–Br1	–37.2 (5)		

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

Table 2

Torsion angles ( $^\circ$ ) in *cis*-stilbenes.

Compound	C4–C3–C1–C2	C14–C9–C2–C1	C3–C1–C2–C9
1,2-dibromo (obs)	144.5 (4)	112.9 (5)	–4.4 (7)
1,2-dibromo (calc)	120	114	0.2
1,2-dichloro (obs)	133.7	111.3	–8.7
1,2-dichloro (calc)	122	115	0.3
4-ClPh-1,2-dichloro (obs)	129.3	128.0	7.1
4-ClPh-1,2-dichloro (calc)	118	115	0.1
<i>cis</i> -stilbene (calc)	121	117	0.1

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999).

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