could easily be constructed without a change of the unit-cell parameters.

It therefore seems that the distortions of the TiO_6 octahedra in $BaTi_2O_5$ are not caused by the bond-strength distribution and cannot be interpreted on electrostatic grounds only. Baur (1961) pointed out that the Ti coordination in $PbTiO_3$ (Shirane, Pepinsky & Frazer, 1956) with Ti–O distances of 1·78, 4×1·98 and 2·38 Å should be described as a 5+1 coordination and a similar distortion of a TiO_6 octahedron in $Na_2Ti_3O_7$ has been interpreted by Andersson & Wadsley (1961) as a tendency of Ti towards 5 coordination. Table 3 gives distances between Ti atoms and their six nearest O neighbours for a number of compounds with Ti in different coordinations. It can be seen that there is no sharp limit between 5 and 6-coordinated Ti. While Ti is clearly 5-coordinated in Y_2TiO_5, fresnoite, and partly in innelite, other Ti atoms in innelite, in $BaTi_2O_5$, $PbTiO_3$ and $Na_2Ti_3O_7$ have a 5+1 coordination.

Table 3. *Distances between titanium atoms and their six nearest oxygen neighbours for a number of compounds with different* Ti *coordinations*

Compound	Bond lengths (Å)
Y_2TiO_5[a]	Ti–O: 1·78, 1·87, 1·91, 2×1·94, 3·89
Fresnoite $Ba_2TiOSi_2O_7$[b]	Ti–O: 1·63, 4×2·00, 3·58
Innelite	Ti(1)–O: 1·62, 1·99, 2·00, 2·05, 2·06, 3·67
$Na_2Ba_3(Ca,Na)(Ba,K,Mn)$	Ti(2)–O: 1·90, 1·92, 2·00, 2·04, 2·09, 2·16
$Ti_3O_4(SO_4)_2(Si_2O_7)_2$[c]	Ti(3)–O: 1·71, 1·93, 1·96, 1·98, 2·01, 3·17
$BaTi_2O_5$[d]	Ti(1)–O: 1·71, 1·87, 2×2·00, 2·06, 2·47
$PbTiO_3$[e]	Ti–O: 1·78, 4×1·98, 2·38
$Na_2Ti_3O_7$[f]	Ti(2)–O: 1·71, 1·87, 1·91, 2×1·94, 2·34

References: (*a*) Mumme & Wadsley (1968); (*b*) Moore & Louisnathan (1969); (*c*) Chernov *et al.* (1971); (*d*) This work; (*e*) Shirane *et al.* (1956); (*f*) Andersson & Wadsley (1961).

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1,6:8,13-Cyclopropanediylidene[14]annulene

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Abstract. $C_{17}H_{12}$, monoclinic, $C2/c$, $Z=8$, $a=19·485\,(3)$, $b=6·812\,(2)$, $c=17·881\,(5)$ Å, $\beta=108·52\,(2)°$, $D_m=1·273$, $D_x=1·277$ g cm^{-3}, m.p. 169–170°C. Mo $K\alpha$ diffractometer data. Final $R=0·054$ on all observed amplitudes. The strain imposed by the bridges of the annulene perimeter and by the cyclopropane ring seem to have a balancing rather than a synergic effect; as a result the annulene ring is nearly planar with bond lengths close to the aromatic value.

Introduction. X-ray diffraction data were measured with Mo $K\alpha$ radiation on a Syntex $P\bar{1}$ four-circle diffractometer equipped with graphite monochromator. Cell dimensions were obtained from 26 reflexions (plus their equivalents) for $\lambda=0·71069$ Å. Systematic absences were hkl for $h+k$ odd, $h0l$ for l odd. A crystal of dimensions 0·30×0·35×0·40 mm was used. Intensities were collected to a maximum 2θ value of 55° (θ–2θ scan mode, scan width $2·1°+\alpha_1\alpha_2$ separation, variable scan speed between 1 and 12° min^{-1}, dead time for coincidence correction $2·1\times10^{-6}$ s). The background was counted for half the total scanning time on each side of the reflexion. Three check reflexions were monitored periodically to test crystal decomposition or movement. Of 2607 measured unique data, 2423 had intensity above background. The variance $\sigma^2(I_{\rm rel})$ was calculated as $[S+B+(0{\cdot}02S)^2]v^2$, with S = scan count, B = total background count and v = scan speed. Lorentz and polarization factors were applied; absorption effects were neglected (μ = 0·8 cm^{-1} for Mo $K\alpha$ radiation). The $N(z)$ test and the statistics on the normalized structure factors were in full agreement with the centric distribution.

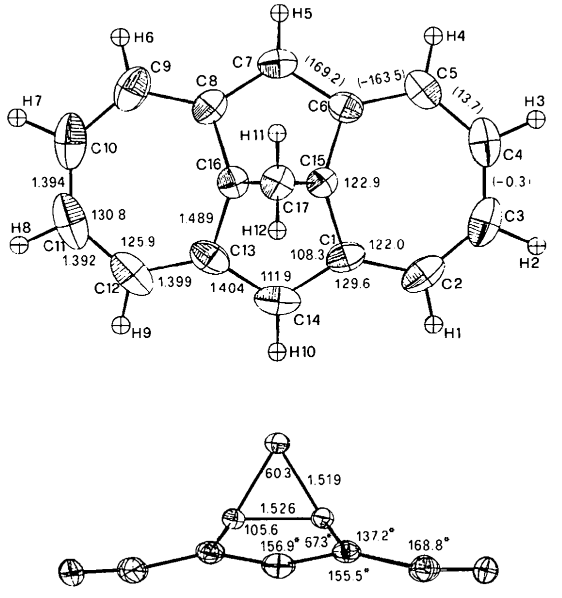

Fig. 1. One molecule of the title compound viewed along two principal axes of inertia. *mm*2-averaged geometric parameters are reported. Bond lengths are corrected for rigid-body motion. Values in parentheses refer to torsion angles, starred values to dihedral angles. Thermal ellipsoids (Johnson, 1965) for carbon atoms are drawn at probabilities 0·40 and 0·20 in the upper and lower part of the figure respectively. Hydrogen atoms are on an arbitrary scale.

The structure was solved by direct methods with the computer programs of Bianchi, Destro & Gavezzotti (1972). After an initial false solution, reassignment of the starting set of reflexions led to an E map where all the 17 carbon atoms were easily recognizable. Refinement on all observed reflexions was by a full-matrix least-squares process on scale factor, extinction parameter [Zachariasen, 1963; Larson, 1967, equation (3); Kerr & Ashmore, 1974, equation (5)], anisotropic carbon and (after the calculation of a difference map) isotropic hydrogen atoms, by minimizing the function $\sum w(|F_o|-|F_c|)^2$ with weights $w=1/\sigma^2(F)$. The program employed was a modified version of *ORFLS* (Busing, Martin & Levy, 1962). Scattering factors for C were obtained from Cromer & Waber (1965) and for H from Stewart, Davidson & Simpson (1965). In the final cycle most shifts were less than 0·1σ, the maximum shift being 0·3σ. $R=\sum||F_o|-|F_c||/\sum|F_o|$ converged to 0·054 for the 2423 observed reflexions (0·061 for all 2607 data), with a goodness of fit $[\sum w(\Delta F)^2/(n-p)]^{1/2}$ = 1·60.* A final difference map showed no significant features, the electron density values being between ±0·30 e Å^{-3}.

The final atomic parameters are listed in Table 1. Bond distances, uncorrected and corrected for rigid-body motion (Schomaker & Trueblood, 1968; program written by Filippini & Gramaccioli, 1969) are reported in Table 2. Bond, torsion, and dihedral angles between least-squares planes are summarized in Fig. 1. Mean values for the e.s.d.'s are 0·003 Å, 0·15° and 0·4° respectively for bond lengths, bond angles and torsion angles involving only C atoms; 0·02 Å for C–H bond lengths and 1° for C–C–H and H–C–H bond angles.

Table 1. *Fractional coordinates and thermal parameters with standard deviations*

The thermal parameters are of the form $\exp[-(B_{11}h^2+2B_{12}hk+\ldots)\times10^{-4}]$.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
C(1)	0·2510 (1)	0·2297 (2)	0·1632 (1)	35 (1)	137 (3)	25 (0)	−5 (1)	9 (0)	3 (1)
C(2)	0·3222 (1)	0·2860 (2)	0·2018 (1)	45 (1)	216 (4)	28 (1)	−32 (1)	5 (0)	−10 (1)
C(3)	0·3838 (1)	0·1976 (3)	0·1950 (1)	29 (1)	363 (5)	35 (1)	−37 (1)	2 (0)	13 (1)
C(4)	0·3929 (1)	0·0182 (3)	0·1626 (1)	22 (0)	390 (5)	40 (1)	0 (1)	8 (0)	24 (1)
C(5)	0·3432 (1)	−0·1270 (3)	0·1280 (1)	29 (1)	272 (4)	38 (1)	19 (1)	14 (0)	11 (1)
C(6)	0·2683 (1)	−0·1077 (2)	0·1039 (1)	27 (0)	184 (3)	25 (0)	7 (1)	11 (0)	−3 (1)
C(7)	0·2148 (1)	−0·2531 (2)	0·0864 (1)	35 (1)	147 (3)	34 (1)	3 (1)	12 (0)	−6 (1)
C(8)	0·1463 (1)	−0·1750 (2)	0·0773 (1)	28 (0)	184 (3)	26 (0)	−12 (1)	7 (0)	3 (1)
C(9)	0·0818 (1)	−0·2715 (3)	0·0714 (1)	34 (1)	247 (4)	41 (1)	−28 (1)	6 (0)	21 (1)
C(10)	0·0207 (1)	−0·1861 (3)	0·0812 (1)	24 (1)	424 (6)	51 (1)	−19 (1)	8 (1)	55 (2)
C(11)	0·0114 (1)	−0·0056 (3)	0·1124 (1)	25 (1)	479 (7)	57 (1)	26 (2)	18 (1)	67 (2)
C(12)	0·0601 (1)	0·1454 (3)	0·1435 (1)	36 (1)	346 (5)	45 (1)	47 (1)	22 (1)	38 (1)
C(13)	0·1288 (1)	0·1648 (2)	0·1359 (1)	32 (0)	190 (3)	32 (1)	28 (1)	15 (0)	24 (1)
C(14)	0·1873 (1)	0·2799 (2)	0·1789 (1)	47 (1)	167 (3)	31 (1)	18 (1)	17 (0)	−1 (1)
C(15)	0·2324 (1)	0·0860 (2)	0·0977 (1)	23 (0)	155 (3)	22 (0)	−3 (1)	8 (0)	1 (1)
C(16)	0·1524 (1)	0·0419 (2)	0·0799 (1)	22 (0)	167 (3)	25 (0)	2 (1)	8 (0)	10 (1)
C(17)	0·1787 (1)	0·1450 (2)	0·0192 (1)	27 (0)	194 (3)	24 (0)	−4 (1)	8 (0)	9 (1)

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* A table of observed and calculated structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 30610 (14 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1 (*cont.*)

	x	y	z	B (Å^2)
H(1)	0·328 (1)	0·392 (3)	0·236 (1)	6·6 (4)
H(2)	0·430 (1)	0·267 (3)	0·223 (1)	7·2 (4)
H(3)	0·444 (1)	−0·016 (2)	0·171 (1)	7·1 (4)
H(4)	0·362 (1)	−0·258 (2)	0·122 (1)	6·2 (4)
H(5)	0·226 (1)	−0·389 (2)	0·087 (1)	5·7 (3)
H(6)	0·080 (1)	−0·410 (3)	0·063 (1)	7·1 (4)
H(7)	−0·023 (1)	−0·273 (2)	0·069 (1)	7·2 (4)
H(8)	−0·036 (1)	0·013 (3)	0·120 (1)	8·4 (4)
H(9)	0·047 (1)	0·241 (2)	0·175 (1)	6·5 (4)
H(10)	0·184 (1)	0·377 (2)	0·216 (1)	6·1 (3)
H(11)	0·179 (1)	0·065 (2)	−0·027 (1)	4·6 (3)
H(12)	0·167 (1)	0·285 (2)	0·009 (1)	4·5 (3)

Table 2. *Bond lengths* (Å)

	Observed	Corrected*		Observed	Corrected
C(1)—C(2)	1·393	1·398	C(6)—C(7)	1·400	1·406
C(5)—C(6)	1·392	1·398	C(7)—C(8)	1·397	1·403
C(8)—C(9)	1·392	1·398	C(13)-C(14)	1·395	1·401
C(12)-C(13)	1·395	1·401	C(1)—C(15)	1·480	1·487
C(2)—C(3)	1·382	1·389	C(6)—C(15)	1·480	1·487
C(4)—C(5)	1·385	1·391	C(8)—C(16)	1·482	1·489
C(9)—C(10)	1·384	1·391	C(13)-C(16)	1·485	1·492
C(11)-C(12)	1·391	1·397	C(15)-C(17)	1·515	1·520
C(3)—C(4)	1·388	1·395	C(16)-C(17)	1·513	1·518
C(10)-C(11)	1·386	1·393	C(15)-C(16)	1·520	1·526
C(14)-C(1)	1·400	1·406			

* After rigid-body correction.

Discussion. This structure determination is part of a study of bridged annulenes for which the chemical behaviour is connected to the strain imposed by the bridges on the annulene perimeter. Accordingly, bond lengths in the annulene ring may range from distances not far from the aromatic value (Gavezzotti, Mugnoli, Raimondi & Simonetta, 1972; Gramaccioli, Mugnoli, Pilati, Raimondi & Simonetta, 1972) to a succession of localized single and double bonds giving rise to olefinic behaviour (Gramaccioli, Mimun, Mugnoli & Simonetta, 1973).

In the case of a single bridge imposed on a [10] annulene derivative it has been shown that the substituents on the bridge play an important role in shifting the equilibrium from the annulene (Gramaccioli & Simonetta, 1971) to the bisnorcaradiene configuration (Bianchi, Morosi, Mugnoli & Simonetta, 1973). In the last case however the bond which closes the cyclopropane ring has an extraordinary length (1·81 Å). In the title compound, which was prepared by Reel & Vogel (1972), the cyclopropane ring is in a different situation and its geometry quite normal. The molecule shows *mm*2 symmetry within experimental error. The C–C distances in the annulene perimeter are in the range 1·389–1·406 Å (values corrected for rigid-body motion; mean 1·398 Å). Torsion angles along the annulene ring show that the misalignment between p_z orbitals of adjacent carbon atoms never exceeds 17°. In comparison with previously determined structures of bridged annulenes (Dobler & Dunitz, 1965; Ganis & Dunitz, 1967; and papers quoted above) the present compound shows the least deviation from planarity for the annulene perimeter, whose atoms are at a distance not more than 0·32 Å from the C(2), C(5), C(9), C(12) plane. In the cyclopropane ring the C(15)–C(16) length (1·526 Å, σ 0·002 Å) is slightly longer than the other two bonds, the difference, however, being only possibly significant. On the whole, it seems that the connexion between C(15) and C(16) by a cyclopropane bridge is the best way to relieve the strain imposed otherwise by the two methylene bridges on the annulene perimeter.

C–H lengths are in the range 0·93–1·01 Å. The shortest intermolecular contacts are between

C(17) in x,y,z and C(17) in $\frac{1}{2}-x$, $\frac{1}{2}-y$, $-z$ (3·38 Å),
C(1) and H(5) in x, $1+y$, z (2·90 Å),
C(13) and H(1) in $\frac{1}{2}-x$, $-\frac{1}{2}+y$, $\frac{1}{2}-z$ (2·86 Å),
H(4) and H(8) in $\frac{1}{2}+x$, $-\frac{1}{2}+y$, z (2·54 Å),
H(2) and H(2) in $1-x$, y, $\frac{1}{2}-z$ (2·60 Å).

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