the conformations of (I) and (II) are such that the formal P=N double bond lies approximately parallel to the P=O bond. This may be compared with $N_3P_3Cl_5$-(N=PPh_3), where the exocyclic P=N bond lies parallel to the phosphazene ring with its multiple-bonded P–N system, but contrasts with geminal $N_3P_3Cl_4Ph$-(N=PPh_3), in which the exocyclic P=N bond lies perpendicular to the phosphazene ring.

In both (I) and (II), the Ph_3P=N groups exhibit the familiar propeller conformation, in which the interplanar angles are 81·7, 96·2 and 117·6° in (I), and 85·8, 98·1 and 79·9° in (II). The absence of short intermolecular contacts in the crystal structures of both compounds suggests that the packing is dominated by van der Waals forces.

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Geometry of the Bicyclo[2.2.2]octatriene System: Crystal Structure of 2,3-(Tetrafluorobenzo)bicyclo[2.2.2]octatriene

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Abstract

$C_{12}H_6F_4$ is monoclinic, space group $C2/c$, with a = 16·10 (1), b = 8·17 (1), c = 14·95 (1) Å, β = 104·71 (5)°, Z = 8. The structure was refined to R = 4·62% for 1173 observed counter amplitudes. E.s.d.'s average 0·004 Å for bond lengths and 0·25° for bond angles not involving H atoms. The bicyclo[2.2.2]-octatriene skeleton deviates to a small but significant extent from its idealized geometry, but maintains *mm*2 symmetry consistent with the overall geometry of the molecule.

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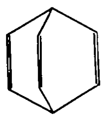
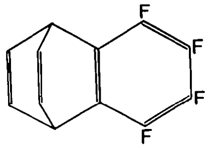
Introduction

The bicyclo[2.2.2]octatriene system (I) has been extensively studied as the tribenzo derivative, triptycene and its substitution products. X-ray analyses of triptycene (Anzenhofer & de Boer, 1970), 1-bromotriptycene (Palmer & Templeton, 1968) and (+)-2,5-dimethoxy-7-dimethylaminotriptycene hydrobromide (Sakabe, Sakabe, Ozeki-Minakata & Tanaka, 1972) have shown that in these molecules the octatriene skeleton approximates closely to its idealized geometry, point group symmetry $\bar{6}m2$ (D_{3h}). However, in the overcrowded molecules 1,2,3,4-tetrachloro-9-*tert*-butyltriptycene (Mikami, Toriumi, Konno & Saito, 1975) and β-chloroethyltriptycene (Karle & Estlin, 1969), significant deviations from ideal geometry occur. We now report the crystal structure of the monobenzo derivative, 2,3-(tetrafluorobenzo)bicyclo[2.2.2]octatriene (II) (Callander, Coe, Tatlow & Uff, 1969) as a further contribution to the study of the bicyclo[2.2.2]octatriene system.


(I)



(II)

Experimental

Crystals were obtained from light petroleum. A crystal 0·5 × 0·3 × 0·3 mm was sealed in a Pantak capillary tube and mounted along the direction of elongation which coincided with *b*. Cell dimensions and intensities were measured on a Stoe two-circle diffractometer with graphite-monochromatized Mo $K\alpha$ radiation. For layers 0–2, 140 counts of 1 s at intervals of 0·01° in ω were taken, backgrounds being measured for 30 s at each end of the scan. For the higher layers (3–9) a variable scan range was employed (Hamor & Hamor, 1978). 2472 reflexions were scanned within the range $0{\cdot}10 < \sin\theta/\lambda < 0{\cdot}65$ Å^{-1} of which 1173 [$I > 2{\cdot}5\sigma(I)$] were considered to be observed. The intensities of three zero-layer reflexions were remeasured after each layer. There was some deterioration of the crystal during the period of data collection and layer scale factors ranging from 1·0 to 1·228 were applied to the intensities to correct for this. Absorption corrections were not applied.

Crystal data

$C_{12}H_6F_4$, M_r = 226·2, monoclinic, a = 16·10 (1), b = 8·17 (1), c = 14·95 (1) Å, β = 104·71 (5)°, U = 1902 Å^3, Z = 8, D_c = 1·580 Mg m^{-3}, $F(000)$ = 912; systematic absences: *hkl*, $h + k$ odd; *h*0*l*, *l* odd; space group *Cc* or *C*2/*c*. *C*2/*c* established as a result of the analysis. Mo $K\alpha$ radiation, λ = 0·71069 Å, μ(Mo $K\alpha$) = 0·099 mm^{-1}.

Structure determination

E statistics indicated the presence of a centre of symmetry and the structure was solved in space group *C*2/*c* by direct methods with *SHELX* (Sheldrick, 1975). Isotropic, full-matrix least-squares refinement reduced *R* from an initial 34% to 14%. The atoms were then allowed to vibrate anisotropically, and after further refinement a difference synthesis gave the positions of all six H atoms. These were included in the refinement with isotropic temperature factors. Refinement was continued until all calculated shifts were $<0{\cdot}05\sigma$ and R = 4·62% for the 1173 observed reflexions. Final atomic coordinates are in Table 1.* The weighting scheme was $w = 1/[\sigma^2(F) + 0{\cdot}00026F^2]$ where $\sigma(F)$ is the e.s.d. in the observed amplitude based on counting statistics.

Computations were carried out on the CDC 7600 computer at the University of Manchester Regional Computer Centre and on the Birmingham University ICL 1906A.

Table 1. *Fractional atomic coordinates* (×10^4) *with e.s.d.'s in parentheses*

	x	*y*	*z*
C(1)	5431 (2)	6960 (3)	4230 (2)
C(2)	5757 (2)	5385 (4)	4261 (2)
C(3)	5237 (2)	4146 (3)	3842 (2)
C(4)	4394 (2)	4468 (3)	3387 (2)
C(5)	3173 (2)	6609 (3)	2857 (2)
C(6)	3319 (2)	7923 (4)	2190 (2)
C(7)	3822 (2)	9112 (4)	2587 (2)
C(8)	4142 (2)	8935 (3)	3629 (2)
C(9)	3354 (2)	8684 (4)	4002 (2)
C(10)	2859 (2)	7491 (4)	3607 (2)
C(11)	4608 (2)	7287 (3)	3769 (2)
C(12)	4074 (2)	6012 (3)	3336 (2)
F(1)	5960 (1)	8153 (2)	4669 (1)
F(2)	6582 (1)	5095 (3)	4702 (1)
F(3)	5545 (1)	2605 (2)	3877 (1)
F(4)	3901 (1)	3193 (2)	2991 (1)
H(5)	2798 (16)	5717 (32)	2554 (18)
H(6)	3036 (20)	7803 (34)	1545 (24)
H(7)	3946 (18)	9998 (38)	2250 (20)
H(8)	4498 (16)	9797 (32)	3933 (17)
H(9)	3256 (17)	9286 (36)	4478 (21)
H(10)	2351 (20)	7132 (33)	3741 (19)

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* Lists of observed and calculated structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34248 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

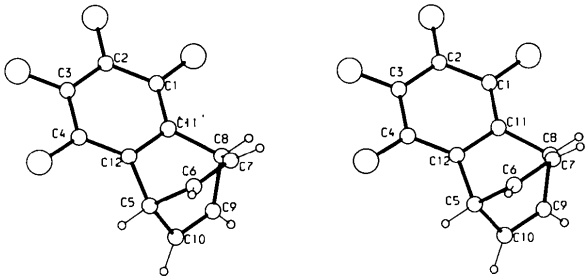

Fig. 1. Stereoscopic view of the molecule showing the atomic labelling.

Results and discussion

Fig. 1 shows a stereoscopic view of the molecule with the atom numbering. F and H atoms take the numbers of the C atoms to which they are attached. Bond lengths, bond angles and selected torsion angles are in Table 2, and the results of mean-plane calculations in Table 3. The thermal parameters of the atoms, except for the H atoms, were analysed for rigid-body thermal motion (Schomaker & Trueblood, 1968). The results are in Table 4, and bond lengths corrected for the effect of libration are listed in Table 2 beside the uncorrected values.

The bicyclo[2.2.2]octatriene system possesses $6m2$ (D_{3h}) symmetry. The title compound, however, because of the unsymmetrical nature of the substitution has only $mm2$ (C_{2v}) symmetry. Bond lengths and angles are generally consistent with this symmetry, and selected mean values are listed in Table 5. Also listed in Table 5 are the corresponding lengths and angles for triptycene (Anzenhofer & de Boer, 1970), 1-bromotriptycene (Palmer & Templeton, 1968), and (+)-2,5-dimethoxy-7-dimethylaminotriptycene hydrobromide (Sakabe, Sakabe, Ozeki-Minakata & Tanaka, 1972). Despite the unsymmetrical substitution of the latter two molecules, the dimensions of the carbon framework of all three approximate to D_{3h} symmetry, and averaging has been carried out accordingly.

Bond lengths in the bicyclo[2.2.2]octatriene system of the title compound deviate from the higher symmetry only inasmuch as C(11)–C(12) which is common to the bicyclo[2.2.2]octatriene skeleton and the benzene ring is significantly longer than the two 'pure' double bonds (1·400 Å as compared with 1·302 and 1·307 Å). The lengths of these two double bonds corrected for thermal libration are 1·311 and 1·316 Å, respectively, still shorter than the standard double-bond length, 1·335 Å (Sutton, 1965). The C–C single bonds are all of type C(sp^3)–C(sp^2) and range from 1·518 to 1·530, mean 1·524 Å, in good agreement with the corresponding lengths in triptycenes (2)–(4) listed in Table 5. The mean corrected length is 1·532 Å, slightly longer than the range of accepted lengths (1·51–1·52 Å) for this type of bond (Dewar & Schmeising, 1960; Pauling, 1960; Sutton, 1965). These values may be compared with the 1·346 and 1·535 Å calculated by Ermer (1974) for the double and single bonds of bicyclo[2.2.2]octatriene with a consistent force field.

Table 2. *Molecular dimensions*

(*a*) Bond lengths (Å) with e.s.d.'s in parentheses (*A*) and bond lengths corrected for thermal libration (*B*)

	A	*B*		*A*	*B*
C(1)–C(2)	1·386 (4)	1·393	C(9)–C(10)	1·302 (4)	1·311
C(2)–C(3)	1·361 (4)	1·371	C(10)–C(5)	1·522 (4)	1·531
C(3)–C(4)	1·379 (4)	1·385	C(1)–F(1)	1·350 (3)	1·359
C(4)–C(12)	1·358 (4)	1·365	C(2)–F(2)	1·345 (3)	1·351
C(11)–C(12)	1·400 (4)	1·410	C(3)–F(3)	1·349 (3)	1·356
C(1)–C(11)	1·356 (4)	1·362	C(4)–F(4)	1·351 (3)	1·361
C(12)–C(5)	1·525 (4)	1·531	C(5)–H(5)	0·981 (27)	
C(5)–C(6)	1·523 (4)	1·532	C(6)–H(6)	0·961 (33)	
C(6)–C(7)	1·307 (5)	1·316	C(7)–H(7)	0·932 (31)	
C(7)–C(8)	1·518 (5)	1·527	C(8)–H(8)	0·948 (26)	
C(8)–C(11)	1·530 (4)	1·537	C(9)–H(9)	0·910 (30)	
C(8)–C(9)	1·524 (4)	1·531	C(10)–H(10)	0·938 (30)	

(*b*) Bond angles (°) with e.s.d.'s in parentheses

C(2)–C(1)–C(11)	120·8 (3)	C(6)–C(5)–H(5)	113·6 (15)
C(2)–C(1)–F(1)	117·9 (3)	C(10)–C(5)–H(5)	114·2 (15)
C(11)–C(1)–F(1)	121·3 (2)	C(12)–C(5)–H(5)	112·3 (14)
C(1)–C(2)–C(3)	119·4 (3)	C(5)–C(6)–C(7)	114·0 (3)
C(1)–C(2)–F(2)	119·9 (3)	C(5)–C(6)–H(6)	118·2 (17)
C(3)–C(2)–F(2)	120·7 (3)	C(7)–C(6)–H(6)	127·7 (17)
C(2)–C(3)–C(4)	119·9 (2)	C(6)–C(7)–C(8)	113·9 (3)
C(2)–C(3)–F(3)	119·9 (3)	C(6)–C(7)–H(7)	121·6 (18)
C(4)–C(3)–F(3)	120·2 (3)	C(8)–C(7)–H(7)	124·5 (18)
C(3)–C(4)–C(12)	121·1 (2)	C(7)–C(8)–C(9)	107·0 (3)
C(3)–C(4)–F(4)	117·6 (2)	C(7)–C(8)–C(11)	104·6 (2)
C(12)–C(4)–F(4)	121·2 (2)	C(9)–C(8)–C(11)	104·9 (2)
C(4)–C(12)–C(11)	119·0 (2)	C(7)–C(8)–H(8)	115·3 (15)
C(4)–C(12)–C(5)	128·8 (2)	C(9)–C(8)–H(8)	112·5 (16)
C(11)–C(12)–C(5)	112·2 (2)	C(11)–C(8)–H(8)	111·8 (15)
C(1)–C(11)–C(12)	119·7 (2)	C(8)–C(9)–C(10)	113·8 (3)
C(1)–C(11)–C(8)	128·7 (2)	C(8)–C(9)–H(9)	122·6 (18)
C(12)–C(11)–C(8)	111·6 (2)	C(10)–C(9)–H(9)	123·5 (18)
C(12)–C(5)–C(6)	104·3 (2)	C(9)–C(10)–C(5)	114·2 (3)
C(12)–C(5)–C(10)	105·0 (2)	C(9)–C(10)–H(10)	127·1 (18)
C(6)–C(5)–C(10)	106·5 (2)	C(5)–C(10)–H(10)	118·7 (17)

(*c*) Selected torsion angles (°); e.s.d.'s *ca* 0·4°

C(11)–C(12)–C(5)–C(6)	56·6	C(6)–C(7)–C(8)–C(9)	−52·8
C(12)–C(5)–C(6)–C(7)	−57·1	C(7)–C(8)–C(9)–C(10)	53·4
C(5)–C(6)–C(7)–C(8)	−0·7	C(9)–C(10)–C(5)–C(6)	−53·2
C(6)–C(7)–C(8)–C(11)	58·1	C(10)–C(5)–C(6)–C(7)	53·7
C(7)–C(8)–C(11)–C(12)	−55·8	C(1)–C(11)–C(12)–C(5)	179·8
C(8)–C(11)–C(12)–C(5)	−0·9	C(1)–C(11)–C(8)–C(7)	123·4
C(11)–C(12)–C(5)–C(10)	−55·2	C(1)–C(11)–C(8)–C(9)	−124·2
C(12)–C(5)–C(10)–C(9)	57·1	C(4)–C(12)–C(11)–C(8)	179·3
C(5)–C(10)–C(9)–C(8)	−0·1	C(4)–C(12)–C(5)–C(6)	−123·5
C(10)–C(9)–C(8)–C(11)	−57·3	C(4)–C(12)–C(5)–C(10)	124·7
C(9)–C(8)–C(11)–C(12)	56·5		

The C–C bonds in the benzene ring show a somewhat anomalous pattern of alternate long and short lengths which is paralleled only in 1-bromotriptycene (3), and is probably not real. The C–F lengths range from 1·351 to 1·361, mean 1·357 Å (corrected) in good agreement with the mean lengths in tetrafluorobiphenyl (1·360) (Goodhand & Hamor, 1978) and 3-methoxypentafluorotropone (1·355) (Hamor & Hamor, 1976), but rather longer than the mean lengths in perfluorobiphenyl (1·344) (Gleason & Britton, 1976)

Table 3. *Mean-plane calculations*

(*a*) Deviations (Å) of atoms from least-squares planes. E.s.d.'s are *ca* 0·003 Å. In the equations of the planes, *x*, *y* and *z* are fractional coordinates relative to the cell axes.

Plane (1): C(1)–C(4), C(11), C(12).

$$8{\cdot}268x + 1{\cdot}334y - 14{\cdot}130z = -0{\cdot}548$$

C(1) 0·010, C(2) −0·006, C(3) −0·003, C(4) 0·008, C(11) −0·004, C(12) −0·005; F(1) 0·033, F(2) −0·026, F(3) −0·002, F(4) 0·026, C(8) −0·037, C(5) −0·017.

Plane (2): C(11), C(12), C(5), C(8).

$$8{\cdot}398x + 1{\cdot}213y - 14{\cdot}129z = -0{\cdot}568$$

C(11) 0·004, C(12) −0·004, C(5) 0·002, C(8) −0·002.

Plane (3): C(5)–C(8).

$$13{\cdot}788x - 4{\cdot}102y - 4{\cdot}988z = 0{\cdot}237$$

C(5) −0·002, C(6) 0·004, C(7) −0·004, C(8) 0·002.

Plane (4): C(5), C(8)–C(10).

$$-5{\cdot}718x + 5{\cdot}210y - 8{\cdot}535z = -0{\cdot}809$$

C(5) 0·000, C(8) 0·000, C(9) −0·001, C(10) 0·001.

(*b*) Dihedral angles (°)

Plane (1)–Plane (2)	1·0
Plane (2)–Plane (3)	118·2
Plane (2)–Plane (4)	118·9
Plane (3)–Plane (4)	122·8

Table 4. *Results of rigid-body-motion analysis*

Tensor of inertia **I**

Eigenvalues	Eigenvectors (reference axes *a*,*b*,*c**)		
549 (at. wt Å²)	−0·6987	0·6463	−0·3066
953	0·4947	0·7462	0·4455
1358	0·5167	0·1595	−0·8412

Libration tensor **L** and translation tensor **T**

	Eigenvalues	Eigenvectors†		
	89×10^{-4} rad²	0·9708	−0·1140	−0·2110
L	48_5	0·2222	0·0962	0·9702
	28	−0·0903	−0·9888	0·1187
	491×10^{-4} Å²	0·8989	−0·2989	0·3204
T	430	0·0132	0·7493	0·6621
	358	−0·4379	−0·5909	0·6775

R.m.s. discrepancy $\langle \Delta U^2 \rangle^{1/2} = 0{\cdot}0034$ Å².

† Referred, in terms of the corresponding direction cosines, to the orthogonal molecular system defined by the eigenvectors of the molecular tensor of inertia **I** with the origin shifted to symmetrize **S**. The components of the origin shift from the molecular centroid are 0·52, 0·08, 0·01 Å.

Table 5. *Comparison of molecular dimensions of benzobicyclo*[2.2.2]*octatrienes*

Bond lengths (uncorrected) and angles have been averaged on the basis of *mm*2 (C_{2v}) symmetry for the title compound (1), and $\bar{6}m2$ (D_{3h}) for compounds (2)–(4). The numbering of the atoms is as shown in Fig. 1. Except where indicated, each listed length or angle is the mean of six values. The maximum deviation from the mean is shown in parentheses in each case.

(1) Present study.
(2) Triptycene (Anzenhofer & de Boer, 1970).
(3) 1-Bromotriptycene (Palmer & Templeton, 1968). The asymmetric unit is ⅓(molecule).
(4) (+)-2,5-Dimethoxy-7-dimethylaminotriptycene hydrobromide (Sakabe *et al.*, 1972).

	(1)	(2)	(3)	(4)
Bond lengths (Å)				
C(5)–C(12)	1·528 (3)[b]	1·534 (15)	1·52 (1)[b]	1·533 (16)
C(5)–C(6)	1·522 (4)[d]			
C(11)–C(12)	1·400[a]	1·402 (12)[c]	1·39[a]	1·405 (8)[c]
C(6)–C(7)	1·305 (3)[b]			
C(1)–C(11)	1·357 (1)[b]	1·395 (18)	1·37 (0)[b]	1·365 (27)
C(1)–C(2)	1·383 (4)[b]	1·383 (10)	$1{\cdot}40_5$ (1_5)[b]	1·395 (24)
C(2)–C(3)	1·361[a]	1·375 (14)[c]	1·35[a]	1·399 (23)[c]
Bond angles (°)				
C(6)–C(5)–C(12)	104·7 (4)[d]	105·3 (8)	107·5 (1)[b]	105·4 (14)
C(6)–C(5)–C(10)	106·8 (3)[b]			
C(4)–C(12)–C(5)	128·8 (1)[b]	127·6 (8)	128·3 (3)[b]	126·2 (12)
C(4)–C(12)–C(11)	119·4 (4)[b]	119·2 (8)	120·3 (4)[b]	120·5 (13)
C(5)–C(12)–C(11)	111·9 (3)[b]	113·1 (10)	111·5 (8)[b]	113·3 (12)
C(5)–C(6)–C(7)	114·0 (2)[d]			
C(2)–C(1)–C(11)	121·0 (2)[b]	119·7 (9)	119·1 (10)[b]	119·6 (16)
C(1)–C(2)–C(3)	119·7 (3)[b]	121·1 (7)	120·7 (5)[b]	119·9 (17)
Flap angles (°) [angles between the mean planes of the four-atom groupings C(5)–(8); C(5), C(8)–(10); C(5), C(8), C(11), C(12)]				
	118·2	119·7	120·0	118·8
	118·9	119·9	120·0	120·0
	122·8	120·4	120·0	121·2

(*a*) Single value, (*b*) mean of two values, (*c*) mean of three values, (*d*) mean of four values.

and 2-nitrononafluorobiphenyl (1·342 Å) (Hamor & Hamor, 1978).

Deviations from D_{3h} symmetry become more apparent from consideration of bond angles. Thus the angles involving the apical bonds of the six-membered ring C(5) to C(10), opposite the tetrafluorobenzo substituent, are significantly larger than the corresponding angles of the other two six-membered rings comprising the octatriene system, which are contiguous with the tetrafluorobenzo substituent (Table 5). These angles average 106·8° for the first ring and 104·7° for the latter two rings. The endocyclic angles at the points of fusion of the benzo substituent are also significantly smaller than the angles at the double bonds, mean values 111·9 and 114·0° respectively. Large distortions from ideal values therefore occur both at the bridgehead C atoms which are formally sp^3-hybridized and more especially at the sp^2-hybridized C atoms of the octatriene system. Similar distortions of bond angle occur in all known triptycene structures (Table 5), irrespective of whether the bicyclo[2.2.2]octatriene system possesses D_{3h} symmetry or not.

The three six-membered rings comprising the octatriene system are boat-shaped with torsion angles (Table 2) close to the expected values ±54, 0° for a standard boat conformation (Bucourt, 1974). The nonzero torsion angles, neglecting signs, in the two rings joined to the benzene ring, range from 55·2 to 58·1, mean 56·7°. The third ring, where the range is 52·8 to

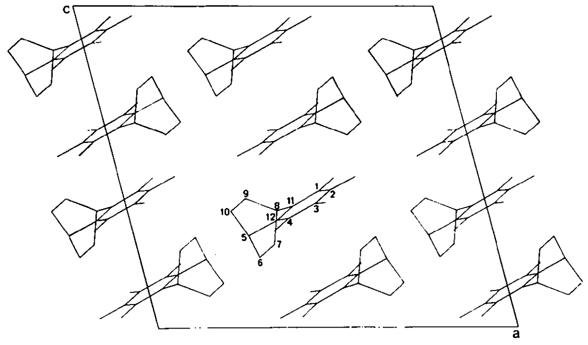

Fig. 2. Projection of the contents of the unit cell along *b*.

Table 6. *The shorter intermolecular contacts* (Å)

E.s.d.'s are *ca* 0·008 Å for distances not involving H.

$H(9)\cdots F(1)^{I}$	2·60	$H(5)\cdots C(9)^{V}$	3·07
$H(6)\cdots F(1)^{II}$	2·73	$F(4)\cdots F(3)^{II}$	3·18
$F(4)\cdots H(7)^{III}$	2·84	$F(2)\cdots C(10)^{VII}$	3·24
$F(3)\cdots H(8)^{III}$	2·86	$F(4)\cdots C(10)^{V}$	3·26
$H(9)\cdots F(2)^{IV}$	2·88	$F(1)\cdots C(9)^{I}$	3·27
$H(5)\cdots C(7)^{V}$	2·88	$F(1)\cdots C(6)^{II}$	3·28
$H(8)\cdots F(1)^{I}$	2·92	$C(1)\cdots C(6)^{II}$	3·37
$H(7)\cdots F(3)^{VI}$	2·96	$F(3)\cdots C(9)^{VII}$	3·38
$F(4)\cdots H(10)^{V}$	2·98	$F(4)\cdots C(7)^{III}$	3·38

Superscripts refer to the following equivalent positions;

(I)	$1-x$,	$2-y$,	$1-z$;	(V)	$\frac{1}{2}-x$,	$y-\frac{1}{2}$,	$\frac{1}{2}-z$;
(II)	$1-x$,	y,	$\frac{1}{2}-z$;	(VI)	$1-x$,	$1+y$,	$\frac{1}{2}-z$;
(III)	x,	$y-1$,	z;	(VII)	$1-x$,	$1-y$,	$1-z$.
(IV)	$x-\frac{1}{2}$,	$\frac{1}{2}+y$,	z;				

53·7, mean 53·3°, is slightly flattened compared with the other two, consistent with the differences in bond angles. A further manifestation of this effect is that the flap angle between the two planes comprising this ring is 122·8° compared with 118·2 and 118·9° for the other two rings. In compounds (2)–(4) which approximate closely to D_{3h} symmetry, the corresponding angles are all close to 120°. The bicyclo[2.2.2]-octatriene system of 1,2,3,4-tetrachloro-9-*tert*-butyltriptycene (Mikami, Toriumi, Konno & Saito, 1975), however, resembles that of the title compound in that the flap angle of the ring opposite the halogenated benzene ring is larger than those of the other two. In this structure and in β-chloroethyltriptycene (Karle & Estlin, 1969) comparatively large distortions of the octatriene system occur due to the bulky substituents at the bridgehead positions, so that detailed comparisons with these structures would not be worthwhile.

Fig. 2 shows the packing of the molecules and Table 6 lists the shorter intermolecular contacts. None of these is substantially shorter than the sum of the corresponding van der Waals radii.

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