in Table 1; bond distances and angles are listed in Table 2.*

Related literature. The title compound has anti-arrhythmic activity. For the preparation and medicinal action see Takagi, Yamazaki & Katoh (1987).

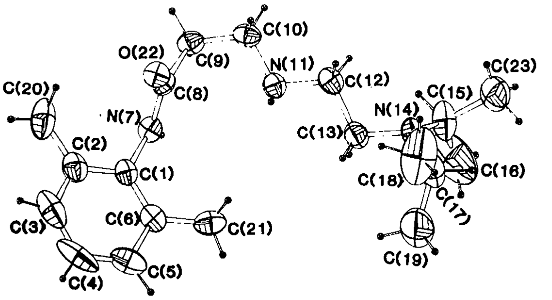

Fig. 1. A perspective view of the molecule with the numbering scheme.

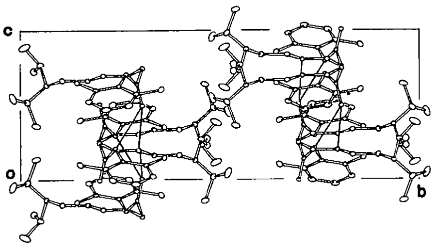

Fig. 2. Crystal structure projected along the *a* axis. Hydrogen bonds are indicated by single lines.

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(1)–C(2)	1·377 (8)	C(9)–C(10)	1·489 (8)
C(1)–C(6)	1·357 (9)	C(10)–N(11)	1·438 (7)
C(1)–N(7)	1·413 (7)	N(11)–C(12)	1·453 (7)
C(2)–C(3)	1·391 (9)	C(12)–C(13)	1·507 (9)
C(2)–C(20)	1·470 (10)	C(13)–N(14)	1·451 (8)
C(3)–C(4)	1·357 (12)	N(14)–C(15)	1·429 (9)
C(4)–C(5)	1·334 (11)	N(14)–C(17)	1·434 (9)
C(5)–C(6)	1·396 (9)	C(15)–C(16)	1·404 (15)
C(6)–C(21)	1·502 (9)	C(15)–C(23)	1·519 (11)
N(7)–C(8)	1·332 (7)	C(17)–C(18)	1·428 (12)
C(8)–C(9)	1·507 (8)	C(17)–C(19)	1·508 (11)
C(8)–O(22)	1·231 (6)		
C(2)–C(1)–C(6)	120·5 (5)	C(9)–C(8)–O(22)	121·3 (5)
C(2)–C(1)–N(7)	118·9 (5)	C(8)–C(9)–C(10)	110·7 (5)
C(6)–C(1)–N(7)	120·6 (5)	C(9)–C(10)–N(11)	110·8 (5)
C(1)–C(2)–C(3)	118·4 (6)	C(10)–N(11)–C(12)	114·1 (4)
C(1)–C(2)–C(20)	123·3 (6)	N(11)–C(12)–C(13)	110·8 (5)
C(3)–C(2)–C(20)	118·3 (6)	C(12)–C(13)–N(14)	111·7 (5)
C(2)–C(3)–C(4)	120·6 (7)	C(13)–N(14)–C(15)	114·6 (5)
C(3)–C(4)–C(5)	120·9 (7)	C(13)–N(14)–C(17)	116·4 (5)
C(4)–C(5)–C(6)	119·9 (7)	C(15)–N(14)–C(17)	115·9 (5)
C(1)–C(6)–C(5)	119·8 (6)	N(14)–C(15)–C(16)	122·1 (7)
C(1)–C(6)–C(21)	120·6 (5)	N(14)–C(15)–C(23)	112·8 (6)
C(5)–C(6)–C(21)	119·6 (6)	C(16)–C(15)–C(23)	108·0 (7)
C(1)–N(7)–C(8)	124·4 (5)	N(14)–C(17)–C(18)	110·0 (7)
N(7)–C(8)–C(9)	116·8 (5)	N(14)–C(17)–C(19)	116·9 (7)
N(7)–C(8)–O(22)	121·9 (5)	C(18)–C(17)–C(19)	107·0 (8)

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* Lists of anisotropic thermal parameters, structure factors, torsion angles, least-squares planes and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44256 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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7,7-Dichloro-4-(diphenylmethylene)bicyclo[3.2.0]hept-2-en-6-one

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Abstract. $C_{20}H_{14}Cl_2O$, $M_r = 341·24$, monoclinic, $P2_1/a$, $a = 9·324$ (1), $b = 18·704$ (3), $c = 9·754$ (1) Å, $\beta = 107·06$ (1)°, $V = 1626·3$ (4) Å^3, $Z = 4$, $D_x = 1·39$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 3·99$ cm^{-1}, $F(000) = 704$, $T = 293$ K, $R = 0·0552$ for 1718 independent observed reflections. The five-membered ring is in an envelope conformation with C(5) the flap. The four-membered ring is folded by 15·9 (6)° along C(1)···C(6). The planes of the two phenyl rings are twisted by 78·4 (7)° and form interplanar angles of

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Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^3)

	x	y	z	U_{eq}*
Cl(1)	3058 (1)	8818 (1)	3633 (1)	69 (1)
Cl(2)	2091 (1)	9826 (1)	5428 (1)	80 (1)
O	2002 (3)	8124 (1)	6404 (2)	53 (1)
C(1)	4911 (4)	9127 (2)	6326 (3)	47 (1)
C(2)	5212 (4)	9598 (2)	7629 (4)	60 (2)
C(3)	5476 (4)	9221 (2)	8833 (4)	52 (2)
C(4)	5389 (4)	8452 (2)	8594 (3)	39 (1)
C(5)	4772 (4)	8370 (2)	6963 (3)	39 (1)
C(6)	3073 (4)	8433 (2)	6298 (3)	40 (1)
C(7)	3259 (4)	9091 (2)	5426 (3)	47 (1)
C(8)	5836 (4)	7941 (2)	9584 (3)	38 (1)
C(11)	5649 (4)	7158 (2)	9254 (3)	40 (1)
C(12)	4355 (4)	6881 (2)	8322 (3)	45 (1)
C(13)	4227 (4)	6156 (2)	8030 (4)	58 (2)
C(14)	5373 (5)	5704 (2)	8661 (4)	69 (2)
C(15)	6665 (5)	5966 (2)	9604 (4)	72 (2)
C(16)	6798 (4)	6690 (2)	9890 (4)	55 (2)
C(21)	6632 (4)	8125 (2)	11108 (3)	43 (1)
C(22)	6115 (4)	7879 (2)	12213 (3)	54 (2)
C(23)	6893 (5)	8029 (2)	13622 (4)	68 (2)
C(24)	8193 (5)	8404 (2)	13947 (4)	71 (2)
C(25)	8720 (4)	8660 (2)	12867 (4)	71 (2)
C(26)	7932 (4)	8522 (2)	11449 (3)	55 (2)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2. *Bond distances* (Å) *and valence angles* (°)

Cl(1)–C(7)	1·778 (3)	Cl(2)–C(7)	1·755 (4)
O–C(6)	1·184 (4)	C(1)–C(2)	1·503 (5)
C(1)–C(5)	1·567 (4)	C(1)–C(7)	1·535 (4)
C(2)–C(3)	1·329 (5)	C(3)–C(4)	1·455 (5)
C(4)–C(5)	1·533 (4)	C(4)–C(8)	1·335 (4)
C(5)–C(6)	1·529 (4)	C(6)–C(7)	1·535 (5)
C(8)–C(11)	1·499 (5)	C(8)–C(21)	1·494 (4)
C(11)–C(12)	1·382 (4)	C(11)–C(16)	1·382 (5)
C(12)–C(13)	1·382 (5)	C(13)–C(14)	1·360 (6)
C(14)–C(15)	1·374 (6)	C(15)–C(16)	1·380 (5)
C(21)–C(22)	1·382 (5)	C(21)–C(26)	1·377 (5)
C(22)–C(23)	1·381 (4)	C(23)–C(24)	1·355 (6)
C(24)–C(25)	1·372 (6)	C(25)–C(26)	1·387 (5)
C(2)–C(1)–C(5)	102·2 (3)	C(2)–C(1)–C(7)	114·6 (3)
C(5)–C(1)–C(7)	90·0 (2)	C(1)–C(2)–C(3)	112·1 (3)
C(2)–C(3)–C(4)	113·3 (3)	C(3)–C(4)–C(5)	104·6 (3)
C(3)–C(4)–C(8)	126·9 (3)	C(5)–C(4)–C(8)	128·4 (3)
C(1)–C(5)–C(4)	105·8 (2)	C(1)–C(5)–C(6)	87·6 (2)
C(4)–C(5)–C(6)	117·3 (3)	O–C(6)–C(5)	136·1 (3)
O–C(6)–C(7)	132·4 (3)	C(5)–C(6)–C(7)	91·5 (3)
Cl(1)–C(7)–Cl(2)	109·9 (2)	Cl(1)–C(7)–C(1)	112·0 (3)
Cl(2)–C(7)–C(1)	118·9 (2)	Cl(1)–C(7)–C(6)	108·6 (2)
Cl(2)–C(7)–C(6)	117·2 (3)	C(1)–C(7)–C(6)	88·6 (2)
C(4)–C(8)–C(11)	123·5 (3)	C(4)–C(8)–C(21)	120·9 (3)
C(11)–C(8)–C(21)	115·5 (3)	C(8)–C(11)–C(12)	122·2 (3)
C(8)–C(11)–C(16)	119·8 (3)	C(12)–C(11)–C(16)	118·0 (3)
C(11)–C(12)–C(13)	120·6 (3)	C(12)–C(13)–C(14)	120·5 (3)
C(13)–C(14)–C(15)	119·9 (4)	C(14)–C(15)–C(16)	119·6 (4)
C(11)–C(16)–C(15)	121·3 (3)	C(8)–C(21)–C(22)	121·0 (3)
C(8)–C(21)–C(26)	120·6 (3)	C(22)–C(21)–C(26)	118·4 (3)
C(21)–C(22)–C(23)	120·4 (4)	C(22)–C(23)–C(24)	120·7 (4)
C(23)–C(24)–C(25)	119·8 (3)	C(24)–C(25)–C(26)	119·8 (4)
C(21)–C(26)–C(25)	120·8 (4)		

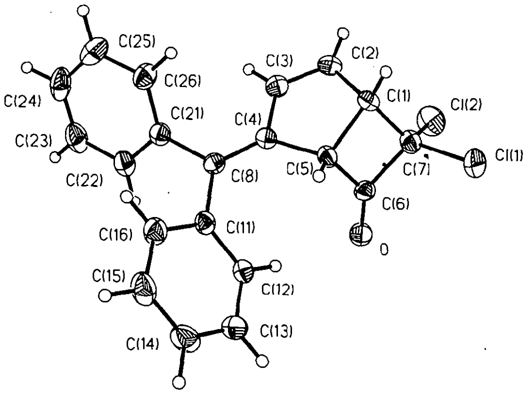
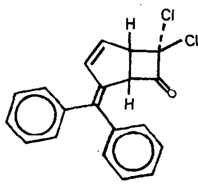


Fig. 1. Drawing of the title compound with thermal ellipsoids shown at the 35% probability level. H atoms are represented by spheres of arbitrary size.

52·6 (7) and 57·9 (7)° with the mean plane of the five-membered ring. The exocyclic double bond is twisted by 7·9 (6)°.



(1)

Experimental. Colorless, transparent crystal of (1), 0·78 × 0·23 × 0·13 mm; Nicolet $R3m/\mu$ update of $P2_1$ diffractometer; data collected in Wyckoff mode ($3 \leq 2\theta \leq 50°$, 2θ fixed, ω varied), scan rate 4 to 29·3° min^{-1}, graphite-monochromated Mo $K\alpha$ radiation; lattice parameters from a least-squares refinement of 25 reflections ($21·91 \leq 2\theta \leq 37·20°$), angles measured by a centering routine; systematic absences ($h0l$, $l = 2n+1$, $0k0$, $k = 2n+1$) consistent with space group $P2_1/a$, Laue symmetry $2/m$; monitored reflections $\bar{2}0\bar{2}$ and $\bar{3}\bar{5}1$ showed only statistical variations in intensities; 2858 independent reflections measured ($0 \leq h \leq 7, 0 \leq k \leq 21, -11 \leq l \leq 11$); $1718 \geq 3·5\sigma(I)$; Lorentz–polarization corrections, ψ-scan empirical absorption correction (transmission factors 0·844 to 0·892); structure solved by direct methods, block-cascade least-squares refinement, H atoms allowed to ride at fixed distance from C atoms with a single isotropic temperature factor refined; final $R = 0·0552$, $wR = 0·0397$ for 209 parameters and 1718 reflections ($R = 0·0999$, $wR = 0·0385$ for all 2858 reflections), $S = 1·537$, $(\Delta/\sigma)_{max} = 0·020$, $(\Delta/\sigma)_{av} = 0·004$; largest peaks in the final difference map of +0·31 and −0·23 e Å^{-3}, $\sum w(|F_o| - |F_c|)^2$ minimized with $w = 1/\sigma^2(F_o)$. All computer programs supplied by Nicolet (Nicolet Instrument Corporation, 1986) for Desktop 30 Microeclipse and Nova 4/C configurations; atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1 lists atomic positional parameters, Table 2 gives interatomic distances and valence angles and Fig. 1 is a drawing of the title compound.*

Related literature. The title compound was prepared from the reaction of diphenylfulvene and dichloroketene (Bartlett & Ando, 1970). The mechanism of hydrolysis of similar compounds to form tropolone derivatives has been reported (Asao, Machiguchi, Kitamura & Kitahara, 1970). Related crystal structures: Friedrichsen, Debaerdemaeker, Bottcher, Hahnemann & Schmidt (1983), Watson & Nagl (1987).

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Structure of Bis(homoadamantane)

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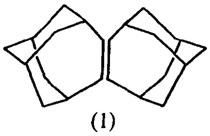
Abstract. 1,2,3,4,5,6,7,8,9,10,11,12,13,14-Tetradecahydro-1,5:3,7:8,12:10,14-tetramethanononalene (eicosene) (1), $C_{20}H_{28}$, $M_r = 268{\cdot}45$, monoclinic, $P2_1/n$, $a = 6{\cdot}593$ (1), $b = 12{\cdot}114$ (2), $c = 9{\cdot}628$ (1) Å, $\beta = 92{\cdot}19$ (1)°, $V = 768{\cdot}4$ Å^3, $Z = 2$, $D_x = 1{\cdot}16$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0{\cdot}60$ cm^{-1}, $F(000) = 296$, $T = 293$ K, $R = 0{\cdot}054$ for 968 unique reflections. The double bond is shielded on the ends by H···H separations of 2·05 (3) Å and on top and bottom by H···H separations ranging from 2·52 (3) to 3·14 (3) Å, which is consistent with the absence of normal olefinic reactivity in the molecule. Molecular-mechanics calculations predict $E_{\rm strain} = 145{\cdot}4$ kJ and $\Delta H_f = -77{\cdot}6$ kJ.



(1)

Table 1. *Atomic coordinates* (×10⁴) *and equivalent isotropic thermal parameters* (Å^2 × 10^3)

	x	y	z	$U_{\rm eq}$*
C(1)	3 (3)	456 (2)	358 (2)	45 (1)
C(2)	−216 (3)	475 (2)	1936 (2)	54 (1)
C(3)	−2267 (4)	36 (2)	2385 (2)	65 (1)
C(4)	−2407 (4)	−1205 (2)	2408 (2)	64 (1)
C(5)	−714 (4)	−1663 (2)	3348 (2)	69 (1)
C(6)	1311 (4)	−1357 (2)	2754 (2)	71 (1)
C(7)	1515 (4)	−108 (2)	2725 (2)	69 (1)
C(8)	−2293 (4)	−1732 (2)	978 (2)	66 (1)
C(9)	1481 (4)	−1885 (2)	1340 (3)	71 (1)
C(10)	−249 (4)	−1587 (2)	315 (2)	56 (1)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

Experimental. Colorless crystal of (1); dimensions 0·45 × 0·28 × 0·30 mm; Nicolet $R3m/\mu$ update of a $P2_1$ diffractometer; data collected in the Wyckoff mode ($3 \le 2\theta \le 50°$, ω varied, 2θ fixed), variable scan speed (4 to 29·3° min^{-1}), monochromated Mo $K\alpha$ radiation; lattice parameters from a least-squares refinement of 25 reflections ($20{\cdot}57 \le 2\theta \le 35{\cdot}35°$), angles measured by a centering routine associated with the diffractometer; systematic absences ($h0l$, $h + l = 2n + 1$; $0k0$, $k = 2n + 1$) consistent with space group $P2_1/n$, Laue symmetry $2/m$; two monitored reflections ($30\bar{1}$ and $0\bar{1}\bar{3}$) showed no statistically significant changes in intensities; 1348 independent reflections measured ($0 \le h \le 7$, $0 \le k \le 14$, $-11 \le l \le 11$) with $968 \ge 3\sigma(I)$; Lorentz–polarization corrections applied, ψ-scan empirical absorption correction (transmission factors 0·903–0·977); direct methods and difference Fourier syntheses revealed the positions of all atoms; block-cascade least-squares refinement with a single thermal parameter for all H atoms; $R = 0{\cdot}0525$, $wR = 0{\cdot}0500$, 968 reflections and 134 parameters, $R = 0{\cdot}0771$ for all

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