

Fig. 2. Packing diagram for (I) viewed down the *b* axis.

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A Neutron Diffraction Study of the Crystal and Molecular Structure of Acenaphthene

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Abstract. $C_{12}H_{10}$, $M_r = 154.2$, orthorhombic, $Pcm2_1$, $a = 8.290$ (4), $b = 14.000$ (7), $c = 7.225$ (4) Å, $V = 838.5$ (7) Å³, $Z = 4$, $D_m = 1.19$, $D_x = 1.221$ (1) Mg m⁻³, 288 K [Ehrlich (1957). *Acta Cryst.* **10**, 699–705]. Neutron diffraction, $\lambda = 1.006$ Å, $\mu = 19.4$ mm⁻¹, $F(000) = 16.96$, room temperature. Final $R(F) = 0.038$ for 668 reflexions [$I > 3\sigma_c(I)$]. The two independent half-molecules are very closely planar with the dimensions of the naphthalene moiety close to those in naphthalene. The corrected length of the aliphatic bond C(7)–C(7') is 1.573 (6) Å. The mean C–H bond lengths are 1.091 (5) Å (aromatic) and 1.133 (7) Å (aliphatic). The results are compared with those of molecular-mechanics calculations.

Introduction. Acenaphthene, or 1,2-dihydroacenaphthylene, is not known to be carcinogenic but the moiety forms a component of several active non-alternant ring systems such as the benzfluoranthenes and the potent carcinogen 3-methylcholanthrene. That the five-membered ring induces some strain was apparent from an early crystal structure analysis (Ehrlich, 1957); twisting of the ethylene bridge occurs in two charge-transfer complexes of acenaphthene (Tickle & Prout, 1973*a,b*) and in *peri*-substituted acenaphthenes (Clough, Kung, Marsh & Roberts, 1976; Tanaka, Kasai, Takenaka & Sasada, 1981). The presence of two crystallographically independent half-molecules in the asymmetric unit makes this noncentrosymmetric

crystal structure valuable for infrared and Raman spectroscopic studies of lattice dynamics (Turković, Colombo, Furić & Kirin, 1974). Splittings in the vibrational spectrum may arise from crystal-field or transition-moment interactions but the calculations require more precisely located H-atom positions (Furić, Colombo, Baranović & Ljucaj, 1979). Accordingly, a neutron-diffraction crystal-structure refinement has been carried out at room temperature.

Experimental. A crystal, bounded by $\{100\}$, $\{010\}$, and $\{001\}$ with dimensions $5.5 \times 2.3 \times 3.0$ mm, sealed to minimize sublimation loss, was mounted on a Huber four-circle diffractometer at the DR3 reactor at the Research Establishment Risø. The crystal was cut from a larger crystal provided by Professor L. Colombo (University of Zagreb). Intensities measured out to $(\sin\theta/\lambda)_{\max} = 0.64 \text{ \AA}^{-1}$ with ω - 2θ scan and Be-monochromatized neutrons of wavelength 1.006 \AA . The scan width (2.2° at $\theta = 0^\circ$ increasing to 4.0° at $\theta = 40^\circ$) was divided into 50 steps. 1059 independent reflexions with $0 \leq h < 10$, $0 \leq k < 17$, $0 \leq l < 9$ gave 668 with $I > 3\sigma(I)$. Standard reflexions 014 and 060 were monitored every 75 reflexions; the mean fall-off in intensity was 0.8%. Intensities integrated using the Lehmann & Larsen (1974) formalism. Data corrected for absorption, transmission factors ranging from 0.56 to 0.66, and for TDS, α ranging from zero for $\sin\theta/\lambda = 0 \text{ \AA}^{-1}$ to 0.3 for $(\sin\theta/\lambda)_{\max}$. [Diffuse X-ray scattering was reported by Ehrlich (1957).] The elastic constants were those determined by Chatterjee & Chakraborty (1981). Least-squares refinement* (on F) included an isotropic extinction parameter, $g = 2.6 (2) \times 10^{-5}$, corresponding to a minimum value of 0.57 for $I/I_{\text{corrected}}$. The weighting scheme was $w = 1/\sigma(F) = \{[\sigma_{\text{cs}}(F^2) + 1.03F^2]^{1/2} - |F|\}^{-1}$, where $\sigma_{\text{cs}}(F^2)$ is the standard deviation from counting statistics. Final $R = 0.038$, $wR = 0.043$, $S = 1.707$, $\Delta/\sigma_{\max} = 0.26$, $\Delta\rho = -0.054 (7)$ to $0.044 (7) \text{ e \AA}^{-3}$. Bond distances were corrected for thermal vibration assuming the carbon skeleton to be a rigid body. The C-H bond distances of the $-\text{CH}_2$ groups were corrected as for riding motion. Computations were carried out on a VAX 11/780 computer with the following programs: *DATAP* and *DSORT* (State University of New York, Buffalo), data processing; *SXTDS1* (Kurittu & Merisalo, 1977), TDS correction; modified *ORFLS* (Busing, Martin & Levy, 1962), least-squares refinement; *TLS* (Schomaker & Trueblood, 1968), rigid-body analysis; *ORFFE* (Busing, Martin & Levy, 1964), geometry and riding-

Table 1. Fractional coordinates and their e.s.d.'s ($\times 10^4$), isotropic thermal parameters, U_{eq} ($\text{\AA}^2 \times 10^{-3}$), and deviations, d ($\text{\AA} \times 10^{-3}$), from the best planes through the carbon atoms

	x	y	z	U_{eq}^\dagger	d
C(1)	4604 (4)	4164 (2)	0	41 (2)	-2 (6)
C(2)	3827 (5)	3295 (3)	-2 (8)	54 (2)	-1 (6)
C(3)	2120 (6)	3271 (3)	-13 (9)	60 (3)	7 (7)
C(4)	1196 (5)	4091 (3)	-6 (10)	58 (2)	1 (7)
C(5)	1963 (7)	5000	12 (11)	47 (3)	-12 (8)
C(6)	3638 (6)	5000	3 (9)	39 (2)	-4 (7)
C(7)	6354 (5)	4437 (3)	-4 (9)	48 (2)	2 (7)
C(11)	2889 (5)	836 (3)	6632 (8)	45 (2)	2 (6)
C(12)	2516 (6)	1705 (3)	5865 (8)	54 (3)	-7 (6)
C(13)	1714 (6)	1727 (3)	4135 (8)	58 (3)	3 (6)
C(14)	1265 (6)	906 (3)	3197 (9)	55 (2)	-1 (6)
C(15)	1636 (7)	0	3967 (9)	44 (3)	5 (6)
C(16)	2430 (7)	0	5668 (9)	40 (3)	-2 (7)
C(17)	3720 (8)	554 (3)	8394 (10)	66 (3)	2 (7)
H(2)	4487 (12)	2628 (6)	-28 (20)	84 (6)	18 (14)
H(3)	1534 (15)	2584 (7)	-61 (24)	92 (7)	41 (18)
H(4)	-141 (13)	4046 (6)	-20 (21)	95 (7)	11 (15)
H(71)	6970 (13)	4158 (8)	-1225 (15)	77 (6)	888 (11)
H(72)	6976 (12)	4171 (8)	1222 (15)	75 (7)	-886 (11)
H(12)	2820 (13)	2372 (6)	6524 (20)	87 (7)	-12 (14)
H(13)	1447 (17)	2412 (7)	3523 (22)	93 (8)	19 (16)
H(14)	641 (13)	954 (8)	1868 (15)	88 (7)	7 (11)
H(171)	3136 (23)	853 (10)	9563 (15)	124 (11)	-830 (11)
H(172)	4941 (19)	831 (8)	8443 (23)	110 (8)	880 (16)

$$\dagger U_{\text{eq}} = \frac{1}{3} \sum_i U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

motion correction; *ORTEP* (Johnson, 1965), drawing; *MMP2* (Burkert & Allinger, 1982), molecular-mechanics calculations. Scattering lengths $b_{\text{C}} = 0.665$, $b_{\text{H}} = -0.374$ pm (Neutron Diffraction Commission, 1972).

Discussion. The asymmetric unit consists of two independent half-molecules, the molecules lying across the crystallographic mirror plane. Final atomic coordinates are listed in Table 1, bond distances and angles in Table 2. The atoms are numbered as Fig. 1. An early X-ray analysis (Kitaigorodsky, 1949) suggested that the aliphatic single bond C(7)–C(7') was unusually long, 1.64 \AA , whereas Ehrlich (1957) found $1.540 (14) \text{ \AA}$. The present neutron diffraction study gives a mean value of $1.573 (6) \text{ \AA}$, which is longer than the usual value for a single bond. Unfortunately, this is the bond for which we find the largest discrepancy between the two independent molecules. In two charge-transfer complexes Tickle & Prout (1973*a,b*) found distances of $1.545 (16)$ and $1.550 (5) \text{ \AA}$. In both cases the ethylene bridge was twisted, a situation which cannot occur in acenaphthene itself, unless there is disorder, as the molecules are across mirror planes. In acenaphthenes where there is substitution of aliphatic hydrogens considerably longer C–C distances of 1.6 \AA or more (Hazell & Hazell, 1977; Gatilov, Nagi, Rybalova & Borodkin, 1984) have been found.

Molecular-mechanics calculations taking electron delocalization into account were carried out using the program *MMP2* (Burkert & Allinger, 1982) to find the minimum-energy conformation of the molecule *in vacuo*, to study the ethylene C–C bond length and its possible variation with twisting of the bridge. The

* Observed and calculated structure factors, anisotropic thermal parameters, H...H distances, and T, L and S values with and without TDS correction have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42734 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

calculated minimum-energy structure (Table 2) has a planar carbon skeleton and the C(7)–C(7') distance is calculated to be 1.561 Å, *i.e.* longer than a normal aliphatic C–C bond, but somewhat though not significantly shorter than the observed one. On the whole, there is reasonable agreement between the molecular-mechanics geometry and that in the crystal. The modification to *MMP2* torsional barriers suggested recently (Liljefors & Allinger, 1985) should not affect our results significantly.

Comparison with neutron diffraction analyses of related compounds, Table 3, shows that generally the

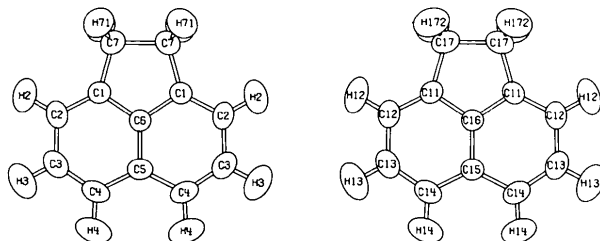


Fig. 1. ORTEP drawings showing the numbering of the atoms for the two independent molecules. H(72) is largely obscured by H(71), as is H(171) by H(172).

aromatic bonds of the naphthalene moiety are similar to those of naphthalene itself, the most obvious difference being the shortening of C(5)–C(6), the bond most likely (Clough, Kung, Marsh & Roberts, 1976) to be affected by strain induced by the five-membered ring. Most of the strain arising from attaching the five-membered ring is taken up by changes in the C–C angles, *e.g.* C(1)–C(6)–C(1') = 111.4 (3)° and C(4)–C(5)–C(4') = 126.8 (4)°. There is very little strain in the naphthalenic C–C–H angles, the largest distortion being for C(1)–C(2)–H(2), C–H being bent 1.6 (5)° away from C(7). The four aliphatic C–H bonds are, after substantial riding-motion corrections, close to the mean of 1.133 (7) Å and significantly longer than the aromatic C–H mean here of 1.091 (5) Å which is similar to that found by neutron diffraction in other polycyclics (*e.g.* Hazell, Jones & Sowden, 1977). The molecule is planar within experimental error. Comparison of thermal parameters from refinements before and after corrections for TDS show that T for the uncorrected data is some 13% too low but that L and S are the same from both data sets. A lack of correction for TDS would thus not have led to errors in bond lengths when correcting for rigid-body motion.

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

Bond distances, *l*, and values, *l*_{corr}, corrected for thermal motion assuming rigid-body motion unless riding motion is indicated (by asterisk), and angles. The weighted mean values for the two independent molecules are compared with the values calculated with *MMP2* and with those of Ehrlich's X-ray determination. E.s.d.'s for the corrected values are assumed to be those of the uncorrected values. Symmetry code: (') *x*, 1 – *y*, *z* for molecule (1), *x*, –*y*, *z* for molecule (2).

	Molecule (1)		Molecule (2)		Weighted average		<i>MMP2</i>	X-ray
	<i>l</i>	<i>l</i> _{corr}	<i>l</i>	<i>l</i> _{corr}	<i>l</i>	<i>l</i> _{corr}	<i>l</i>	<i>l</i>
C(1)–C(2)	1.377 (5)	1.382	1.372 (6)	1.378	1.375 (4)	1.380	1.373	1.373 (12)
C(1)–C(6)	1.418 (4)	1.423	1.414 (5)	1.420	1.416 (3)	1.422	1.409	1.406 (12)
C(2)–C(3)	1.416 (6)	1.421	1.416 (6)	1.424	1.416 (3)	1.423	1.428	1.433 (13)
C(3)–C(4)	1.380 (6)	1.385	1.385 (7)	1.391	1.382 (5)	1.388	1.383	1.350 (12)
C(4)–C(5)	1.423 (5)	1.428	1.419 (5)	1.425	1.421 (4)	1.427	1.427	1.417 (14)
C(5)–C(6)	1.389 (7)	1.394	1.394 (7)	1.402	1.391 (5)	1.398	1.392	1.398 (13)
C(1)–C(7)	1.501 (5)	1.506	1.500 (7)	1.509	1.501 (4)	1.507	1.507	1.524 (13)
C(7)–C(7')	1.576 (8)	1.582	1.552 (10)	1.558	1.567 (6)	1.573	1.561	1.540 (14)
C(2)–H(2)	1.082 (11)	1.086	1.078 (11)	1.083	1.080 (8)	1.085	1.102	
C(3)–H(3)	1.078 (11)	1.082	1.079 (12)	1.084	1.078 (8)	1.083	1.103	
C(4)–H(4)	1.110 (12)	1.114	1.092 (12)	1.099	1.101 (8)	1.107	1.103	
C(7)–H(71)	1.092 (11)	1.132*	1.059 (15)	1.140*	1.080 (9)	1.135	1.115	
C(7)–H(72)	1.090 (12)	1.126*	1.084 (18)	1.143*	1.089 (10)	1.131	1.115	
	Molecule (1)	Molecule (2)	Weighted average	<i>MMP2</i>	X-ray			
C(2)–C(1)–C(6)	117.7 (4)	118.3 (4)	118.0 (3)	118.4	118.6 (7)			
C(1)–C(2)–C(3)	119.2 (4)	118.8 (4)	119.0 (3)	118.3	118.4 (7)			
C(2)–C(3)–C(4)	122.4 (4)	122.7 (5)	122.5 (3)	122.6	121.9 (7)			
C(3)–C(4)–C(5)	119.7 (4)	119.4 (4)	119.6 (3)	120.0	121.5 (7)			
C(4)–C(5)–C(4')	126.9 (5)	126.7 (6)	126.8 (4)	128.7	128.0 (7)			
C(4)–C(5)–C(6)	116.6 (3)	116.6 (3)	116.6 (2)	115.6	116.0 (7)			
C(1)–C(6)–C(1')	111.3 (4)	111.7 (5)	111.4 (3)	109.8	112.4 (7)			
C(1)–C(6)–C(5)	124.4 (2)	124.1 (2)	124.2 (1)	125.1	123.8 (7)			
C(2)–C(1)–C(7)	132.6 (3)	132.8 (4)	132.7 (2)	130.7	132.8 (7)			
C(6)–C(1)–C(7)	109.6 (3)	108.9 (4)	109.3 (2)	110.8	108.6 (7)			
C(1)–C(7)–C(7')	104.8 (2)	105.2 (2)	105.0 (1)	104.3	105.2 (6)			
C(1)–C(2)–H(2)	121.8 (7)	122.5 (8)	122.1 (5)	120.5				
C(3)–C(2)–H(2)	119.0 (7)	118.7 (9)	118.9 (6)	121.2				
C(2)–C(3)–H(3)	118.1 (8)	118.5 (10)	118.3 (6)	118.5				
C(4)–C(3)–H(3)	119.5 (8)	118.8 (10)	119.2 (6)	118.9				
C(3)–C(4)–H(4)	120.5 (6)	120.4 (6)	120.5 (4)	120.2				
C(5)–C(4)–H(4)	119.8 (6)	120.1 (6)	120.0 (4)	119.8				
C(1)–C(7)–H(71)	111.2 (7)	111.3 (10)	111.2 (6)	109.9				
C(1)–C(7)–H(72)	111.6 (7)	111.3 (8)	111.5 (5)	109.9				
C(7')–C(7)–H(71)	111.0 (6)	113.2 (8)	111.8 (5)	111.5				
C(7')–C(7)–H(72)	110.0 (6)	111.0 (6)	110.5 (4)	111.5				
H(71)–C(7)–H(72)	108.3 (8)	105.1 (13)	107.4 (7)	109.5				

Table 3. Mean bond lengths (Å) in acenaphthene compared with those in acenaphthylene, fluoranthene, and naphthalene as determined by neutron diffraction

	Acenaphthene ^a	Acenaphthylene ^b	Fluoranthene ^c	Naphthalene ^d	Naphthalene ^e
C(1)–C(2)	1.380 (4)	1.381 (7)	1.361 (5)	1.373 (3)	1.381 (2)
C(2)–C(3)	1.423 (4)	1.424 (8)	1.433 (6)	1.410 (3)	1.421 (2)
C(3)–C(4)	1.388 (4)	1.382 (8)	1.383 (6)	1.373 (3)	1.381 (2)
C(4)–C(5)	1.427 (3)	1.433 (6)	1.415 (5)	1.423 (3)	1.426 (2)
C(5)–C(6)	1.398 (5)	1.386 (10)	1.413 (6)	1.420 (3)	1.432 (2)
C(1)–C(6)	1.422 (3)	1.441 (6)	1.415 (5)	1.423 (3)	1.426 (2)
C(1)–C(7)	1.507 (4)	1.466 (7)	1.498 (4)		
C(7)–C(7')	1.573 (6)	1.395 (11)	1.408 (6)		

Notes: (a) this work, (b) 80 K, Wood, Welberry & Rae (1985), (c) Hazell, Jones & Sowden (1977), (d) Hazell (1980, unpublished, cited in Hazell & Mariezcurrena, 1980); new refinement with the data of Pawley & Yeats (1969), (e) 12 K, Natkaniec, Belushkin, Dyck, Fuess & Zeyen (1983).

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Structure of (±)-2-(2-Chloro-3,4-dimethoxyphenyl)-2-hydroxy-N-isopropylethylamine Hydrochloride

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Abstract. $C_{13}H_{21}ClNO_3 \cdot Cl^-$, $M_r = 310.2$, triclinic $P\bar{1}$, $a = 7.580$ (4), $b = 8.566$ (5), $c = 12.346$ (6) Å, $\alpha = 82.57$ (2), $\beta = 101.26$ (2), $\gamma = 94.91$ (2)°, $V = 778.1$ (7) Å³, $Z = 2$, $D_m = 1.33$ (1), $D_x = 1.324$ Mg m⁻³, $\lambda(Mo K\alpha) = 0.71069$ Å, $\mu = 0.420$ mm⁻¹, $F(000) = 328.0$, $T = 298$ K. Final $R = 0.048$ for 1619 observed reflections. The main conformational features of the molecule are similar to those mostly observed for structurally related β -adrenergics. The molecular packing is determined by