ausgeprägte Neigung der Substanz zur Zwillingsbildung erklären. Spiegelt man die Struktur, wie in Fig. 3 geschehen, an der (100)-Ebene und translatiert um *b*/2, dann bleiben an den Grenzflächen der Zwillingspartner nur noch die Schichten parallel (100) erhalten. Die Kontaktabstände zwischen diesen Schichten an den Grenzflächen sind hier nur unwesentlich verschieden von denjenigen zwischen analogen Schichten im unverzwillingten Kristall. Sie sind nur in wenigen Fällen 0,2 bis 0,3 Å kürzer. Es tritt innerhalb einer Translationsperiode in *b* jeder Kontaktabstand doppelt auf, im unverzwillingten Kristall symmetriebedingt und an der Grenzfläche zwischen zwei Zwillingspartnern verursacht durch eine exakte *b*/2-Translation. Bei einer von *b*/2 verschiedenen Translation würde einer der äquivalenten Kontaktabstände grösser, der andere kleiner, was für die gewählte Translation spricht. Aus den angeführten Kriterien kann man schliessen, dass die Packungsdichte durch die Zwillingsbildung an der Grenzfläche kaum geändert wird.

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8-Benzoyl-5-ethoxy-1-naphthol

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Abstract. $C_{19}H_{16}O_3$, orthorhombic, $Pbc2_1$, a = 10·488 (9), b = 17·815 (13), c = 7·944 (6) Å, Z = 4, D_m = 1·29, D_x = 1·30 Mg m^{-3}. The structure was solved by direct methods and refined by the full-matrix least-squares technique to an R value of 0·042 (R_w = 0·043, w = 1) for 1130 reflections with $\sin\theta/\lambda \leq 0·56$ Å^{-1}. The molecules form intermolecular hydrogen bonds.

Introduction. The title compound was obtained by the reaction of 2-phenyl-5*H*-naphtho[1,8-*bc*]furan-5-one with acid in ethanol. This reaction was of interest in the investigation of heterocyclic 12-π- and 14-π-systems. The structure determination was undertaken to find out the molecular constitution and the hydrogen-bonding scheme.

Dark-brown needle-shaped crystals were obtained by recrystallization of the compound from an acetone–water solution. A single crystal of approximate dimensions 0·26 × 0·20 × 0·18 mm (μ = 0·70 mm^{-1} for Cu $K\alpha$) was used. Systematic absences were $0kl$ for k odd and $h0l$ for l odd. Of the space groups $Pbcm$ and $Pbc2_1$, the latter was chosen on the basis of the statistical distribution of the E values and from packing considerations. This assumption was verified by the final results.

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Table 1. *Final positional parameters*

(*a*) Fractional atomic coordinates of the non-hydrogen atoms (× 10^4) with their standard deviations in parentheses

	x	*y*	*z*
C(1)	8565 (4)	5804 (2)	7321 (8)
C(2)	8491 (5)	6571 (3)	7523 (8)
C(3)	7907 (5)	7011 (3)	6277 (9)
C(4)	7397 (5)	6696 (3)	4861 (8)
C(5)	7028 (5)	5564 (3)	3095 (8)
C(6)	7200 (5)	4821 (3)	2827 (8)
C(7)	7815 (5)	4381 (3)	4024 (8)
C(8)	8240 (4)	4673 (2)	5528 (8)
C(9)	8092 (4)	5450 (2)	5826 (8)
C(10)	7490 (4)	5910 (2)	4611 (8)
C(11)	5980 (5)	5740 (3)	443 (8)
C(12)	5405 (5)	6399 (3)	−525 (10)
C(13)	8940 (4)	4136 (2)	6659 (8)
C(14)	8277 (4)	3770 (2)	8099 (8)
C(15)	8975 (5)	3330 (3)	9211 (9)
C(16)	8364 (6)	2943 (3)	10483 (9)
C(17)	7055 (6)	2989 (3)	10640 (9)
C(18)	6450 (5)	3426 (3)	9559 (10)
C(19)	6950 (5)	3823 (3)	8277 (9)
O(1)	9067 (3)	5333 (2)	8487 (6)
O(5)	6437 (4)	6049 (2)	2007 –
O(13)	10025 (3)	3944 (2)	6293 (6)

(*b*) Fractional atomic coordinates (× 10^4) of the hydrogen atoms

H(2)	8851	6811	8553
H(3)	7865	7567	6429
H(4)	6960	7018	4003
H(6)	6883	4589	1759
H(7)	7952	3834	3783
H(111)	5313	5351	665
H(112)	6701	5515	−206
H(121)	5237	6243	−1714
H(122)	6015	6831	−505
H(123)	4585	6556	12
H(15)	9922	3293	9090
H(16)	8868	2631	11288
H(17)	6614	2700	11548
H(18)	5404	3457	9694
H(19)	6440	4142	7487
H(O1)	9487	5654	9356

Table 2. *Bond distances* (Å) *and angles* (°), *with standard deviations in parentheses*

C(1)–C(2)	1·377 (7)	C(9)–C(1)–C(2)	120·9 (5)
C(1)–O(1)	1·357 (7)	C(9)–C(1)–O(1)	115·3 (4)
C(1)–C(9)	1·434 (8)	O(1)–C(1)–C(2)	123·8 (5)
C(2)–C(3)	1·404 (9)	C(1)–C(2)–C(3)	119·8 (5)
C(3)–C(4)	1·367 (9)	C(2)–C(3)–C(4)	121·4 (5)
C(4)–C(10)	1·417 (7)	C(3)–C(4)–C(10)	119·6 (5)
C(5)–O(5)	1·370 (12)	C(6)–C(5)–C(10)	120·5 (5)
C(5)–C(6)	1·353 (7)	C(10)–C(5)–O(5)	114·2 (6)
C(5)–C(10)	1·437 (9)	C(6)–C(5)–O(5)	125·3 (7)
C(6)–C(7)	1·391 (8)	C(5)–O(5)–C(11)	117·0 (5)
C(7)–C(8)	1·378 (9)	C(5)–C(6)–C(7)	120·4 (6)
C(8)–C(9)	1·412 (6)	C(6)–C(7)–C(8)	121·9 (5)
C(8)–C(13)	1·505 (7)	C(7)–C(8)–C(9)	118·8 (5)
C(9)–C(10)	1·416 (8)	C(7)–C(8)–C(13)	115·8 (4)
C(11)–O(5)	1·441 (15)	C(9)–C(8)–C(13)	125·2 (5)
C(11)–C(12)	1·527 (8)	C(8)–C(9)–C(10)	120·1 (5)
C(13)–O(13)	1·222 (6)	C(8)–C(9)–C(1)	122·2 (5)
C(13)–C(14)	1·489 (8)	C(10)–C(9)–C(1)	117·7 (4)
C(14)–C(15)	1·389 (8)	C(5)–C(10)–C(9)	118·3 (4)
C(14)–C(19)	1·402 (7)	C(9)–C(10)–C(4)	120·5 (5)
C(15)–C(16)	1·380 (9)	C(4)–C(10)–C(5)	121·2 (5)
C(16)–C(17)	1·381 (9)	O(5)–C(11)–C(12)	105·8 (5)
C(17)–C(18)	1·376 (9)	C(8)–C(13)–O(13)	119·3 (5)
C(18)–C(19)	1·390 (9)	C(8)–C(13)–C(14)	120·6 (4)
		C(14)–C(13)–O(13)	119·7 (5)
		C(13)–C(14)–C(15)	119·3 (4)
		C(13)–C(14)–C(19)	120·8 (5)
		C(19)–C(14)–C(15)	119·8 (5)
		C(14)–C(15)–C(16)	120·2 (5)
		C(15)–C(16)–C(17)	119·9 (6)
		C(16)–C(17)–C(18)	120·7 (6)
		C(17)–C(18)–C(19)	120·2 (5)
		C(18)–C(19)–C(14)	119·2 (5)

The diffraction data were collected with a Picker FACS-I automatic diffractometer, fitted with a graphite monochromator and using Cu $K\alpha$ radiation (λ = 1·5418 Å). Cell parameters were determined by a least-squares fit to the angular settings of 15 reflections. The cell parameters were in agreement with those determined by Auer (1976) using Weissenberg and precession methods. The intensity of the reflections was measured by the θ–2θ scan method with a stationary counter for the background. The data were collected in the region $4 \leq 2\theta \leq$ 118°; two reflections were taken as standards, and measured after every 48 observations.

Averaging over symmetrically equivalent reflections yielded 1158 reflections of which 1078 were classified as observed [$I_{\text{obs}} > 3\sigma(I)$]. The intensities were reduced to a set of structure amplitudes by application of the Lorentz–polarization corrections. No absorption or extinction corrections were applied.

MULTAN (Germain, Main & Woolfson, 1971) was used to determine the phases of 170 reflections, $|E| \geq$ 1·6. An E map based on the set of phases with the highest combined figure of merit revealed the positions of all non-hydrogen atoms. Three cycles of least-squares calculations with isotropic thermal parameters reduced R to 0·096 and another three cycles with anisotropic thermal parameters gave R = 0·076. All H atoms could be located in the difference Fourier syntheses but they were included in their idealized positions (C–H = 1·00 Å). In the following two cycles of least-squares refinement the non-hydrogen atoms were refined with anisotropic temperature factors. To reduce the number of free parameters in the refinement, the H atoms were constrained to their ideal positions with the equivalent isotropic thermal parameters of the bonded atoms. The final R value was 0·042 (R_w = 0·043, w = 1).* The atomic coordinates are listed in Table 1, bond lengths and angles in Table 2 and the equation of best planes and deviations of the atoms in Table 3. The

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33905 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

scattering factors were those of Cromer & Mann (1968) for non-hydrogen atoms and those of Stewart, Davidson & Simpson (1965) for H.

Discussion. The result of the structure determination and the numbering scheme are illustrated in Fig. 1. The C–C bond distances within the naphthol group range from 1·353 to 1·437 Å, thus deviating considerably from the ideal value of 1·396 Å for aromatic bonding (Kitaigorodsky, 1973). The other bond distances are quite normal. The angle of tilt between the least-squares planes defined by the rings of the naphthol group is 4·0°. The plane fitted to the C atoms of the phenyl ring forms an angle of 86·8° with the plane fitted to the C atoms of the naphthol rings (*cf.* Table 3), contradicting a centrosymmetric space group, where the molecules would have to lie on mirror planes. The molecule at (x,y,z) is bonded to the molecule at $(2-x,\ 1-y,\ \frac{1}{2}+z)$ by a hydrogen bond O(1)–H(O1)···O(13′) of 2·745 Å [H(O1)···O(13′) = 1·77 Å]. The 2_1 axis produces a symmetrically equivalent hydrogen bond between the molecules (x,y,z) and $(2-x,\ 1-y,\ -\frac{1}{2}+z)$ thus forming a chain along the c direction. There are no other intermolecular contact distances which are shorter than the sums of the corresponding van der Waals atomic radii.

All calculations were performed on a Univac 1108 computer at the Rechenzentrum der Universität Karlsruhe. We wish to thank Professor Dr H. Wondratschek for his interest in this work. One of us (GDN) would like to acknowledge the award of a senior Humboldt fellowship from the Alexander von Humboldt-Stiftung.

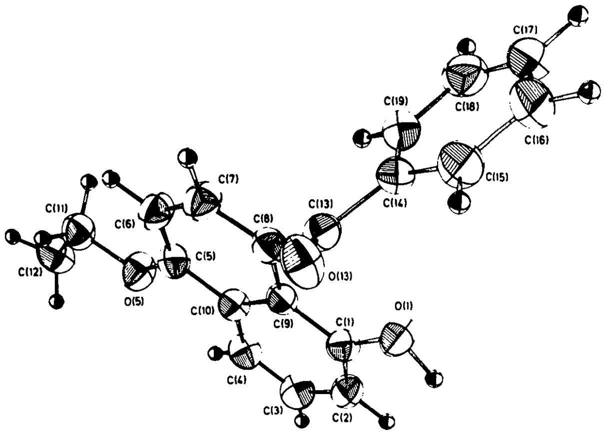

Fig. 1. Perspective view (Johnson, 1965) of the molecule with the labelling of atoms.

Table 3. *Least-squares planes and deviations of the atoms from these planes* (Å)

The equations of the planes are expressed in the form $PX + QY + RZ = S$, where X, Y and Z are the coordinates in Å relative to the orthogonal axes and S is the distance from the origin to the plane. Asterisks indicate atoms included in the calculation of the plane.

Plane 1: plane fitted to C atoms of the naphthol group

$$0{\cdot}8828X + 0{\cdot}1510Y - 0{\cdot}4448Z = 6{\cdot}9391$$

Plane 2: plane fitted to C atoms of the phenyl group

$$0{\cdot}1095X + 0{\cdot}7848Y + 0{\cdot}6100Z = 10{\cdot}1505$$

Angle φ of tilt between the planes 1 and 2: $\varphi = 86{\cdot}8°$

Plane 1 Atoms	Δ (Å)	Plane 2 Atoms	Δ (Å)
C(1)	−0·035*	C(14)	−0·004*
C(2)	0·032*	C(15)	0·000*
C(3)	0·050*	C(16)	0·005*
C(4)	−0·007*	C(17)	−0·005*
C(5)	−0·029*	C(18)	0·001*
C(6)	0·025*	C(19)	0·004*
C(7)	0·053*	O(5)	0·018
C(8)	−0·006*	O(13)	−0·436
C(9)	−0·040*		
C(10)	−0·044*		
C(11)	−0·015		
C(12)	−0·028		
C(13)	0·098		
O(1)	−0·108		
O(5)	−0·061		

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