Mean distances for different types of bonds are: $C(sp^3)$–$C(sp^3)$ = 1·535; $C(sp^2)$–$C(sp^2)$ = 1·389; $C(sp^2)$–$N(sp^2)$ = 1·390; and $C(sp^2)$–$N(sp^3)$ = 1·453 Å.

Short contacts between non-bonded atoms are typical van der Waals interactions.

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8,8′-Biquinolyl

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Abstract. $C_{18}N_2H_{12}$, monoclinic, $P2_1/a$, $Z=4$, M.W. 256·3; $a=8·668$ (3), $b=19·967$ (10), $c=7·686$ (5) Å, $\beta=103·36$ (4)°; $D_x=1·315$, $D_m=1·30$ g cm^{-3}; final $R=0·034$. The sp^2–sp^2 single bond between the two ring systems has a length of 1·495 (2) Å. The configuration is *trans*, the angle between the two halves of the molecule being 96·8°.

Introduction. The colourless, compact prismatic crystals were supplied by Dr J. Pedersen (Department of Organic Chemistry, Chalmers University of Technology). A specimen, 0·6 × 0·4 × 0·6 mm, was mounted on a Syntex $P2_1$ four-circle diffractometer. A θ–2θ time variable scan technique was used, $2\theta_{max}$ being 100°, with a scan speed varying between 2·0 and 12·0° min^{-1}. Graphite-monochromatized Cu $K\alpha$ radiation ($\lambda=1·5418$ Å) was used to measure 1448 reflexions, of which 1369 were retained when an observed–unobserved cut-off at $4·0\sigma(I)$ was employed. The systematic absences, $0k0$, $k=2n+1$, and $h0l$, $h=2n+1$, uniquely determined the space group as $P2_1/a$. The intensities were reduced to structure factors by application of Lorentz and polarization factors, but no absorption correction was made.

The structure was solved by direct methods with *MULTAN* (Main, Lessinger, Woolfson, Germain & Declercq, 1974). With 200 normalized structure factors ($E_{min}=1·49$) and 1600 $\sum_2$ relationships, sixteen sets of phases were generated. The map computed with the most consistent set showed all twenty non-hydrogen atoms as well as four spurious peaks, the latter at a considerably lower level. Block-diagonal least-squares refinement of the non-hydrogen atoms with isotropic temperature factors gave an R of 0·084. The H atoms, located from geometric considerations, were included in the further refinements. Anisotropic temperature factors were introduced for the N and C atoms, and weights were calculated from $w=(12+|F_o|+0·025\times|F_o|^2)^{-1}$. The final R was 0·034 for 1369 reflexions (0·036 with 79 unobserved reflexions included) when 230 parameters were refined. The scattering factors were those of Doyle & Turner (1968) for C and N, and those of Stewart, Davidson & Simpson (1965) for H. The final atomic positions and thermal parameters are given in Table 1.*

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31704 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

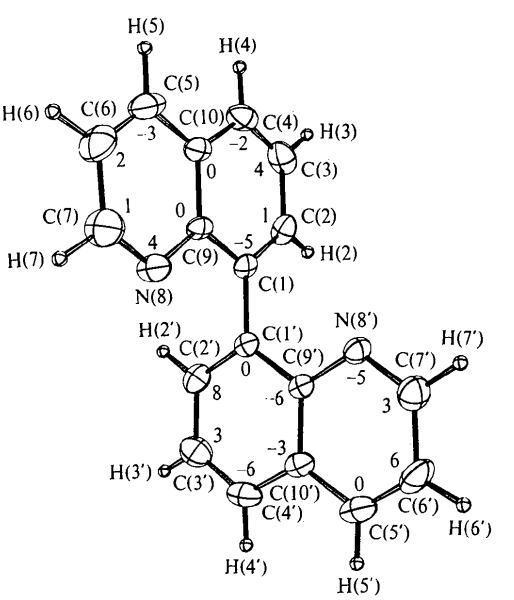

Fig. 1. The molecular structure of 8,8′-biquinolyl with the deviations in Å (× 10^3) from the least-squares planes noted.

Discussion. The present investigation was undertaken in connexion with stereochemical investigations performed by Pedersen (1975), in order to determine accurate values of bond distances and angles by crystallographic methods.

The structural features of 8,8′-biquinolyl are shown in Fig. 1 (*ORTEP*: Johnson, 1965). The molecule consists of two halves, linked by an sp^2–sp^2 single bond. The two halves, which are chemically identical, are crystallographically independent and thus the bond distances are determined twice. Corresponding values show excellent agreement (Table 2). The estimation of the standard deviations seems to be correct in view of the sizes of the discrepancies.

C(1) and C(1′) are linked by an sp^2–sp^2 single bond of 1·495 (2) Å. This is significantly longer than the corresponding length in related compounds, *e.g.* in 1,1′-binaphthyl, 1·475 (5) (Kerr & Robertson, 1969); in the α form of perylene, 1·471 (5) (Camerman & Trotter, 1964); and in a perylene–fluoranil complex,

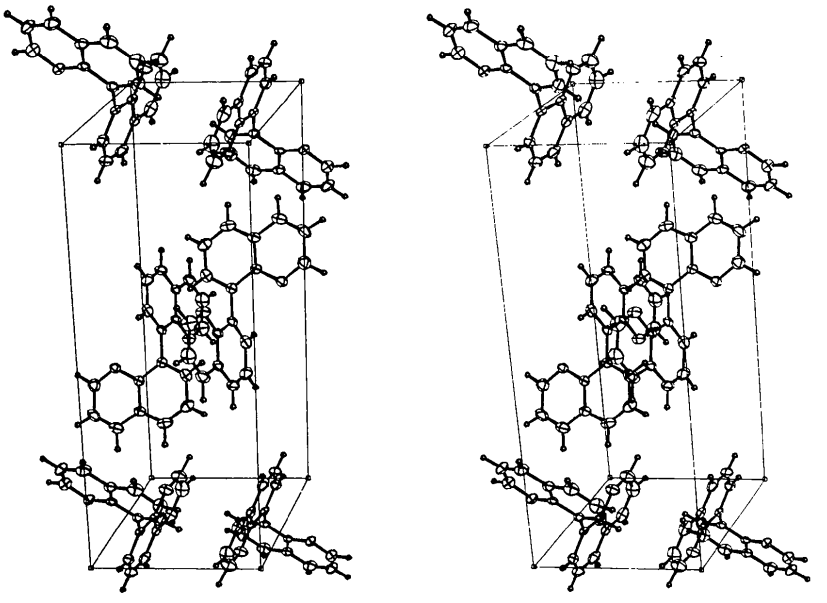

Fig. 2. Stereo view showing the molecular packing.

Table 1. *Positional and thermal parameters for* 8,8′*-biquinolyl*

Non-hydrogen parameters have been multiplied by 10^5 (positional) and 10^4 (thermal). Hydrogen positional parameters have been multiplied by 10^3. The form of the anisotropic thermal ellipsoid is $\exp[-2\pi^2(U_{11}h^2a^{*2}+\ldots+U_{23}klb^*c^*)]$.

	x	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	69126 (20)	54548 (8)	77558 (22)	275 (9)	163 (9)	193 (9)	−58 (16)	100 (16)	−129 (15)
C(2)	63763 (22)	48708 (9)	83215 (24)	355 (10)	283 (10)	319 (10)	−172 (18)	291 (19)	−119 (17)
C(3)	73291 (27)	42910 (9)	85977 (25)	662 (14)	176 (10)	335 (11)	−154 (20)	223 (21)	3 (17)
C(4)	88102 (25)	43031 (9)	83047 (24)	563 (12)	207 (10)	289 (10)	233 (20)	50 (20)	−97 (17)
C(5)	109483 (23)	49383 (10)	73746 (25)	329 (10)	435 (12)	342 (11)	385 (20)	−11 (19)	−131 (19)
C(6)	114406 (23)	55222 (11)	68011 (28)	232 (9)	611 (14)	483 (12)	111 (21)	203 (20)	7 (22)
C(7)	104110 (24)	60690 (10)	65643 (29)	340 (11)	413 (13)	594 (13)	−72 (20)	284 (22)	105 (22)
N(8)	89744 (17)	60630 (7)	68495 (21)	244 (8)	239 (8)	497 (9)	−33 (14)	285 (16)	74 (15)
C(9)	84563 (20)	54736 (8)	74290 (21)	291 (9)	165 (9)	213 (9)	18 (16)	59 (16)	−93 (15)
C(10)	94188 (22)	48929 (9)	77074 (22)	341 (10)	231 (10)	180 (9)	133 (17)	4 (17)	−133 (15)
C(1′)	58975 (20)	60685 (8)	74391 (22)	190 (8)	202 (8)	287 (10)	−88 (15)	183 (17)	−11 (15)
C(2′)	50624 (23)	62221 (10)	57549 (24)	355 (10)	356 (11)	288 (10)	−15 (19)	171 (19)	−138 (17)
C(3′)	40980 (24)	67978 (10)	53936 (26)	361 (11)	413 (12)	371 (11)	142 (20)	−5 (20)	134 (19)
C(4′)	39797 (22)	72191 (9)	67277 (27)	284 (9)	259 (10)	527 (12)	117 (18)	151 (20)	155 (19)
C(5′)	47671 (23)	75107 (10)	99446 (27)	376 (10)	228 (10)	558 (11)	84 (18)	366 (21)	−87 (20)
C(6′)	56089 (25)	73566 (10)	115917 (26)	563 (12)	281 (11)	437 (11)	−31 (20)	428 (22)	−329 (18)
C(7′)	65337 (24)	67714 (9)	118405 (25)	448 (11)	335 (11)	334 (10)	−61 (20)	221 (20)	−123 (18)
N(8′)	66384 (18)	63549 (7)	105506 (18)	323 (8)	237 (8)	265 (8)	−3 (14)	171 (15)	−78 (13)
C(9′)	57937 (19)	65056 (8)	88623 (22)	155 (8)	168 (9)	302 (9)	−104 (15)	198 (16)	−43 (15)
C(10′)	48293 (20)	70871 (9)	84938 (24)	221 (8)	194 (9)	395 (10)	−51 (16)	243 (18)	−33 (17)

Table 1 (*cont.*)

	x	*y*	*z*	*B*
H(2)	538 (2)	486 (1)	853 (2)	1·5 (3)
H(3)	696 (2)	389 (1)	902 (3)	4·3 (5)
H(4)	952 (2)	393 (1)	846 (2)	3·1 (4)
H(5)	1164 (2)	455 (1)	760 (2)	2·9 (4)
H(6)	1250 (2)	556 (1)	655 (3)	4·3 (5)
H(7)	1078 (3)	650 (1)	611 (3)	4·8 (5)
H(2′)	516 (2)	595 (1)	480 (2)	2·5 (4)
H(3′)	348 (3)	686 (1)	418 (3)	4·8 (5)
H(4′)	330 (2)	762 (1)	651 (2)	3·6 (4)
H(5′)	409 (2)	789 (1)	964 (2)	4·0 (5)
H(6′)	561 (2)	761 (1)	1261 (3)	4·3 (5)
H(7′)	716 (2)	665 (1)	1308 (2)	3·0 (4)

1·473 (5) Å (Hanson, 1963). There appears to be no π contribution to this bond. The quinoline residues are planar, with an angle of 96·8° between them. Fig. 2 shows the molecular packing.

In addition to the computer programs already mentioned the following were used: *BLOCK* for least squares (Lindgren); *DATAP*1 for data reduction (Lindgren); *DISTAN* for distances and angles (Zalkin); and *PLANEFIT* for fitting of least-squares planes (Wengelin).

We thank Dr J. Pedersen for supplying the crystals and suggesting the problem. Thanks are also due to Dr John Wood for revising the English text. This work has been supported by the Swedish Natural Science Research Council (Contract No. 2318).

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

C(1)—C(2)	1·363 (2)	C(1′)—C(2′)	1·364 (3)
C(2)—C(3)	1·409 (3)	C(2′)—C(3′)	1·411 (3)
C(3)—C(4)	1·354 (3)	C(3′)—C(4′)	1·348 (3)
C(4)—C(10)	1·410 (3)	C(4′)—C(10′)	1·412 (3)
C(10)–C(5)	1·410 (3)	C(10′)–C(5′)	1·410 (3)
C(5)—C(6)	1·350 (3)	C(5′)—C(6′)	1·343 (3)
C(6)—C(7)	1·395 (3)	C(6′)—C(7′)	1·405 (3)
C(7)—N(8)	1·313 (3)	C(7′)—N(8′)	1·313 (2)
N(8)—C(9)	1·370 (2)	N(8′)—C(9′)	1·368 (2)
C(9)—C(10)	1·416 (2)	C(9′)—C(10′)	1·420 (2)
C(1)—C(1′)	1·495 (2)		
C(2)—H(2)	0·91 (2)	C(2′)—H(2′)	0·93 (2)
C(3)—H(3)	0·94 (2)	C(3′)—H(3′)	0·97 (2)
C(4)—H(4)	0·96 (2)	C(4′)—H(4′)	0·99 (2)
C(5)—H(5)	0·96 (2)	C(5′)—H(5′)	0·95 (2)
C(6)—H(6)	0·98 (2)	C(6′)—H(6′)	0·93 (2)
C(7)—H(7)	1·01 (2)	C(7′)—H(7′)	1·01 (2)

C(1)—C(2)—C(3)	121·3 (2)
C(2)—C(3)—C(4)	120·4 (2)
C(3)—C(4)—C(10)	120·6 (2)
C(4)—C(10)—C(9)	118·8 (2)
C(10)—C(9)—C(1)	119·9 (2)
C(9)—C(1)—C(2)	119·0 (2)
C(9)—C(10)—C(5)	117·8 (2)
C(10)—C(5)—C(6)	119·8 (2)
C(5)—C(6)—C(7)	118·5 (2)
C(6)—C(7)—N(8)	125·0 (2)
C(7)—N(8)—C(9)	117·2 (2)
N(8)—C(9)—C(10)	121·8 (2)
C(1′)—C(2′)—C(3′)	122·0 (2)
C(2′)—C(3′)—C(4′)	120·3 (2)
C(3′)—C(4′)—C(10′)	120·0 (2)
C(4′)—C(10′)–C(9′)	119·8 (2)
C(10′)–C(9′)—C(1′)	119·2 (2)
C(9′)—C(1′)—C(2′)	118·6 (2)
C(9′)—C(10′)–C(5′)	117·4 (2)
C(10′)–C(5′)—C(6′)	119·8 (2)
C(5′)—C(6′)—C(7′)	119·2 (2)
C(6′)—C(7′)—N(8′)	124·1 (2)
C(7′)—N(8′)—C(9′)	117·5 (2)
N(8′)—C(9′)—C(10′)	122·0 (2)

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