phthalide was also confirmed to be in the *Z* form (Joshi, Hegde, Rogers & Williams, 1980).

The two molecules in the asymmetric unit do possess a pseudo twofold axis of rotation (0·53, y^+, 0·32) with the rotation axis about 18° away from the *b* axis. The relationship between molecules *A* and *B* is shown in Fig. 1 as the projection along this y^+ axis. The numbers listed on the atoms of *A* are the differences in the *y* coordinates of the two independent molecules. Therefore, the two independent molecules are very similar, but cannot pack to give higher symmetry.

Of course, this study cannot completely rule out the possibility of a different conformation in solution, but the rotation around the C=C double bond must go through a very high energy barrier. Therefore, the conformation in the solution state (NMR data) and that of the solid state are assumed to be the same.

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4-Acetyl-3′-chlorobiphenyl, $C_{14}H_{11}ClO$

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Abstract. $M_r = 230·7$, monoclinic, $P2_1/c$, $a = 3·88$ (1), $b = 9·03$ (1), $c = 32·82$ (5) Å, $\beta = 98·5$ (2)°, $V = 1137·26$ Å^3, $Z = 4$, $D_m = 1·29$, $D_x = 1·35$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1·5418$ Å, $\mu = 2·627$ mm^{-1}, $F(000) = 480$, $T = 293$ K, $R = 0·068$ for 1212 observed densitometer and visually measured equi-inclination Weissenberg data. The average C–C bond length in the phenyl rings is 1·391 Å. The molecule is non-planar; the angle between the phenyl rings is 37·7 (3)° and the acetyl group is rotated about its C–C bond by 4·1 (2)°. The C–Cl bond is 1·745 (6) Å and makes an angle of 1·3 (2)° with the phenyl plane.

Introduction. The structure determination of the title compound forms part of an investigation into liquid-crystal compounds and their chemical precursors.

Experimental. D_m measured by flotation in aqueous cadmium *n*-dodecatungstoborate. Thin transparent needle crystals, 0·3 × 0·08 × 0·05 and 0·1 × 0·1 × 0·06 mm, respectively, for *a*- and *b*-axis Weissenberg data. 1600 reflexions measured on a Joyce–Loebl flying-spot densitometer from multiple-film photographs using Cu $K\alpha$ radiation. Data merged to give 1212 unique observed reflexions; h −3→3, k 0→11, l 0→40; $R_{int} = 0·05$. Structure solved by Patterson synthesis and refined (on *F*) by block-diagonal least squares with anisotropic thermal parameters for the non-hydrogen atoms. H-atom positions, initially obtained from a difference synthesis and placed at geometrically reasonable positions, refined with isotropic thermal parameters. Final $R = 0·068$, unit weights used. $(\Delta/\sigma)_{max}$ in final refinement cycle 0·009 for positional and 0·004 for thermal parameters. Max. and min. heights in final $\Delta\rho$ map +0·31 and −0·27 e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Computer programs used: *SHELX*76 (Sheldrick, 1976) and locally written programs supplied by HHS and Drs C. Morgan and M. J. Mottram.

Discussion. Table 1* gives atomic parameters and Table 2 bond lengths and angles. The atomic numbering is shown in Fig. 1.

The phenyl rings are planar to within ±0·01 Å with an average C–C bond length of 1·391 Å. In several 2′ and 3′ halogen-substituted biphenyls the halogen atom has been found to be displaced out of the plane of the

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, intermolecular distances and details of mean-plane calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42052 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Fractional coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^3$) *with e.s.d.'s in parentheses*

$U_{eq} = (U_{11}U_{22}U_{33})^{1/3}$.

	x	y	z	U_{eq}
Cl	3699 (5)	−2928 (2)	2705 (1)	62 (1)
C(1)	955 (15)	−1945 (7)	1517 (2)	42 (4)
C(2)	2280 (15)	−1848 (7)	1933 (2)	42 (3)
C(3)	1884 (16)	−3047 (7)	2187 (2)	45 (4)
C(4)	201 (17)	−4336 (7)	2048 (2)	51 (4)
C(5)	−1184 (17)	−4410 (8)	1633 (2)	56 (5)
C(6)	−821 (16)	−3239 (8)	1364 (2)	51 (4)
C(7)	1397 (14)	−684 (7)	1234 (2)	38 (4)
C(8)	2134 (16)	−955 (7)	834 (2)	47 (4)
C(9)	2689 (18)	202 (8)	580 (2)	51 (4)
C(10)	2620 (16)	1672 (7)	719 (2)	44 (4)
C(11)	1887 (16)	1940 (7)	1112 (2)	49 (4)
C(12)	1277 (16)	782 (8)	1364 (2)	46 (4)
C(13)	3432 (19)	2908 (8)	442 (3)	61 (5)
C(14)	3996 (18)	2619 (8)	50 (2)	54 (4)
O	3532 (23)	4324 (8)	602 (2)	129 (6)

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

C(1)–C(2)	1·390 (8)	C(8)–C(9)	1·373 (10)
C(1)–C(6)	1·411 (9)	C(9)–C(10)	1·405 (10)
C(1)–C(7)	1·495 (9)	C(10)–C(13)	1·502 (10)
C(2)–C(3)	1·389 (9)	C(10)–C(11)	1·382 (9)
C(3)–Cl	1·745 (6)	C(11)–C(12)	1·376 (9)
C(3)–C(4)	1·380 (9)	C(7)–C(12)	1·395 (9)
C(4)–C(5)	1·390 (10)	C(13)–C(14)	1·361 (11)
C(5)–C(6)	1·398 (10)	C(13)–O	1·381 (11)
C(7)–C(8)	1·406 (9)		

C(1)–C(2)–C(3)	118·9 (6)	C(8)–C(7)–C(12)	118·2 (6)
C(2)–C(3)–C(4)	123·2 (6)	C(7)–C(8)–C(9)	120·4 (6)
C(2)–C(3)–Cl	118·2 (5)	C(8)–C(9)–C(10)	120·7 (6)
C(4)–C(3)–Cl	118·6 (5)	C(9)–C(10)–C(11)	118·9 (6)
C(3)–C(4)–C(5)	117·4 (6)	C(9)–C(10)–C(13)	119·4 (6)
C(4)–C(5)–C(6)	121·5 (6)	C(11)–C(10)–C(13)	121·7 (6)
C(5)–C(6)–C(1)	119·5 (6)	C(10)–C(11)–C(12)	120·5 (6)
C(6)–C(1)–C(2)	119·4 (6)	C(11)–C(12)–C(7)	121·3 (6)
C(6)–C(1)–C(7)	120·3 (5)	C(10)–C(13)–C(14)	120·5 (7)
C(2)–C(1)–C(7)	120·2 (5)	C(10)–C(13)–O	117·0 (7)
C(1)–C(7)–C(8)	120·3 (6)	O–C(13)–C(14)	122·5 (7)
C(1)–C(7)–C(12)	121·3 (5)		

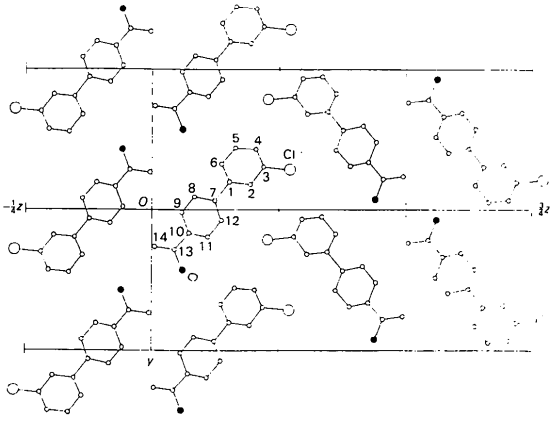

Fig. 1. The arrangement of the molecules in the unit cell viewed along **a**.

ring; the Cl atom in the present structure is displaced by 0·040 (5) Å, the C(3)–Cl bond being inclined at 1·3 (2)° to the phenyl ring. A similar angle of 1·4 (4)° for the C(3)–F bond was found in 3′-fluorobiphenyl-4-carboxylic acid (Sutherland & Rawas, 1983). The C(3)–Cl bond of 1·745 (6) Å is in agreement with the value 1·738 (10) Å in 4-acetyl-2′-chlorobiphenyl (Sutherland & Hoy, 1968) and longer than the value 1·723 (10) Å in 3-chlorobiphenyl-4-carbontrile (Sutherland & Rawas, 1984). C(1) is displaced by 0·082 (9) Å, C(13) by 0·066 (19) Å from the phenyl ring C(7)–C(12). The angle between the phenyl rings, φ_1, of 37·7 (3)° is similar to the values of 38·6 and 36·3 (6)° determined in 4-acetyl-3′-bromobiphenyl (Sutherland & Hoy, 1969) and 3′-fluorobiphenyl-4-carboxylic acid respectively. The axis of the molecule defined by C(1), C(4), C(7), C(10) deviates signficantly from collinearity. Not only is there a rotation φ_1 about the C(1)–C(7) bond but also three other rotations; $\varphi_2 = 1·0$ (2)° of the ring C(1)–C(6) about an axis in its plane through C(1) perpendicular to C(1)–C(7); and $\varphi_3 = 3·1$ (2)°, the corresponding angle of rotation for ring C(7)–C(12); $\varphi_4 = 4·1$ (0·2)° between the mean plane of the phenyl ring C(7)–C(12) and the acetyl group. Similar values for φ_2, φ_3 and φ_4 of 1·2, 4·1 and 2·9° respectively were determined in 4-acetyl-3′-bromobiphenyl.

The acetyl groups form non-bonded dimers across centres of symmetry in the cell, C(14)···O being 3·705 (10) Å. This was also a feature of the structures of 4-acetyl-3′-bromobiphenyl and 4-acetyl-2′-chlorobiphenyl. Considerable difficulty was experienced in distinguishing C(14) and O and a second data set from different crystals gave similar results. The C(13)–C(14) and C(13)–O bond lengths are respectively shorter and longer than the normally accepted values. Interchanging C(14) and O produced no difference and it is felt that there is disorder in the structure. Similar bond lengths and angles for the acetyl group were found in 4-acetyl-3′-bromobiphenyl.

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