Discussion. The refined positional parameters are in Table 1* and bond distances and angles in Table 2. A view of the molecule along **b** is shown in Fig. 1.

The aromatic ring is, as usual, planar. The ring C(1)–C(6)–C(7)–C(8)–C(11)–O(2) has a boat conformation. In the four-membered ring C(8)–C(9)–C(10)–C(11), only one of the angles deviates from 90° by more than 2σ. The ring junction H atoms, H(8) and H(11), are *cis*. The stereochemistry is thus similar to that previously assigned to the photocycloaddition products of substituted ethylenes to chromones (Hanifin & Cohen, 1969).

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond lengths involving H and mean-planes' calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42619 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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4′-Nitro-2-biphenylamine

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Abstract. $C_{12}H_{10}N_2O_2$, $M_r = 214{\cdot}2$, monoclinic, $C2/c$, $a = 20{\cdot}66\ (5)$, $b = 7{\cdot}86\ (3)$, $c = 13{\cdot}29\ (1)$ Å, $\beta = 104{\cdot}6\ (2)°$, $V = 2088$ Å^3, $Z = 8$, $D_m = 1{\cdot}37$, $D_x = 1{\cdot}36$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 0{\cdot}69$ mm^{-1}, $F(000) = 896$, $T = 290$ K, $R = 0{\cdot}102$ for 1175 observed reflexions. The average C–C bond in the phenyl rings is 1·391 Å. The molecule is non-planar; the angle between the phenyl rings is 54·7 (6)°, the angle between the nitro group and the ring to which it is bonded is 7·1 (6)° and the bond N–C(4′) is 1·453 (9) Å.

Introduction. The structure determination of 4′-nitro-2-biphenylamine forms part of an investigation into liquid-crystal compounds and their chemical precursors.

Experimental. D_m measured by flotation in aqueous cadmium *n*-dodecatungstoborate; orange opaque crystals, 0·6 × 0·02 × 0·05 mm and 0·45 × 0·016 × 0·004 mm, respectively, for *b*-axis, $k = 0$–6 and *c*-axis *hk*0 Weissenberg data. 1221 reflexions measured from multiple-film photographs, Cu $K\alpha$ radiation: $-26 \le h \le 24$; $0 \le k \le 6$; $0 \le l \le 16$. Data merged to give 1175 unique observed reflexions; $R_{int} = 0{\cdot}06$; structure solved by direct methods with *SHELX*76 (Sheldrick, 1976) and refined by least squares (F values) with anisotropic thermal parameters for non-hydrogen atoms. H-atom positions, initially obtained from difference synthesis and placed at geometrically reasonable positions, refined with isotropic thermal parameters; $R = 0{\cdot}102$; unit weights. $(\Delta/\sigma)_{max}$ in final refinement cycle 0·03 for positional and 0·04 for thermal parameters. Max. and min. heights in final $\Delta\rho$ map +0·30 and −0·40 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 ring with the attached amino group is planar to within ±0·004 Å; in the other phenyl ring deviations of up to ±0·01 Å from the mean plane occur. The average C–C bond in the two rings is 1·391 Å. The C(1)–C(7) bond length, 1·465 (9) Å, although slightly shorter than in some biphenyl com-

* Lists of structure factors, anisotropic thermal parameters, H atom parameters, intermolecular contact distances and mean-plane calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42634 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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pounds is not significantly shorter than the theoretical value of 1·477 Å. The C(4)–N(1) bond, 1·453 (9) Å, is shorter than the value 1·475 (4) Å in 4-acetyl-2′-nitrobiphenyl (Sutherland, Hogg & Williams, 1974) and somewhat shorter than the 1·468 (9) Å in 2′-nitro-4-biphenylamine, but is very similar to 1·457 (2) Å in 7-nitro-2-fluorenylamine (Fallon & Ammon, 1974). The length appears to be related to the rotation, φ_4, about the C–N bond. In 4-acetyl-2′-nitrobiphenyl and 2′-nitro-4-biphenylamine, the angle of rotation, due to steric effects, is 45·6 and 34·6°, respectively, whereas in the present structure it is 7·1 (6)° and in 7-nitro-2-fluorenylamine it is 5·7°. The N(1)–O(1) and N(2)–O(2) bonds of 1·224 (8) and 1·231 (7) Å are comparable with the values quoted in other nitro-substituted compounds (Sakore & Pant, 1966; Sakore, Tavale & Pant, 1967).

Table 1. *Fractional atomic coordinates* (×10⁴) *and equivalent isotropic thermal parameters* (Å² ×10³) *with e.s.d.'s in parentheses*

	x	*y*	*z*	U_{eq}*
C(1)	4193 (3)	3602 (9)	3640 (4)	37 (4)
C(2)	4876 (3)	4010 (9)	3829 (5)	47 (4)
C(3)	5360 (3)	2760 (10)	3941 (5)	43 (4)
C(4)	5156 (3)	1078 (9)	3852 (5)	40 (4)
C(5)	4491 (3)	612 (8)	3651 (5)	42 (4)
C(6)	4019 (3)	1886 (10)	3566 (5)	46 (4)
C(7)	3693 (3)	4956 (9)	3521 (5)	43 (4)
C(8)	3675 (3)	6224 (10)	2765 (5)	49 (4)
C(9)	3208 (4)	7512 (10)	2587 (6)	58 (5)
C(10)	2739 (4)	7552 (11)	3167 (6)	60 (5)
C(11)	2730 (3)	6335 (11)	3918 (6)	59 (5)
C(12)	3212 (3)	5015 (10)	4093 (5)	49 (4)
N(1)	5655 (3)	−259 (10)	3972 (4)	52 (4)
N(2)	3192 (3)	3798 (10)	4849 (5)	79 (5)
O(1)	5471 (3)	−1737 (8)	3811 (4)	66 (4)
O(2)	6249 (3)	142 (8)	4257 (5)	74 (4)

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

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

C(1)–C(2)	1·407 (8)	C(1)–C(7)	1·465 (9)
C(2)–C(3)	1·382 (10)	C(7)–C(8)	1·410 (9)
C(3)–C(4)	1·383 (10)	C(8)–C(9)	1·377 (10)
C(4)–C(5)	1·383 (9)	C(9)–C(10)	1·381 (10)
C(5)–C(6)	1·382 (9)	C(10)–C(11)	1·386 (11)
C(4)–N(1)	1·453 (9)	C(11)–C(12)	1·416 (10)
N(1)–O(1)	1·224 (8)	C(12)–C(7)	1·395 (8)
N(1)–O(2)	1·231 (7)	C(12)–N(2)	1·396 (9)
C(1)–C(6)	1·392 (10)		
C(1)–C(2)–C(3)	121·5 (7)	C(7)–C(8)–C(9)	122·3 (6)
C(2)–C(3)–C(4)	118·3 (6)	C(8)–C(9)–C(10)	118·7 (7)
C(3)–C(4)–C(5)	122·4 (6)	C(9)–C(10)–C(11)	121·7 (7)
C(4)–C(5)–C(6)	118·0 (6)	C(10)–C(11)–C(12)	119·2 (7)
C(5)–C(6)–C(1)	122·1 (6)	C(11)–C(12)–C(7)	120·2 (7)
C(3)–C(4)–N(1)	119·3 (6)	C(11)–C(12)–N(2)	118·3 (6)
C(5)–C(4)–N(1)	118·2 (6)	C(7)–C(12)–N(2)	121·5 (6)
C(4)–N(1)–O(1)	119·1 (6)	C(12)–C(7)–C(8)	118·0 (6)
C(4)–N(1)–O(2)	118·3 (7)	O(1)–N(1)–O(2)	122·6 (7)
C(1) C(7)–C(12)	123·1 (6)	C(2)–C(1)–C(7)	120·2 (6)
C(1)–C(7)–C(8)	118·8 (6)	C(6)–C(1)–C(7)	122·2 (6)
C(2)–C(1)–C(6)	117·6 (6)		

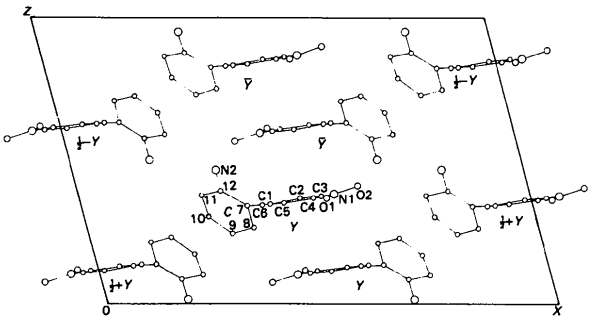

Fig. 1. The arrangement of the molecules in the unit cell viewed along **b**.

The planarity of biphenyl derivatives can be distorted by steric interaction of crystal packing. The angle between the rings about the central C–C bond, φ_1, of 54·7 (6)° is smaller than the 57·1° in 2′-nitro-4-biphenylamine, but larger than the 45·9 (2)° in 4-acetyl-2′-nitrobiphenyl. It is larger than that observed in 2′-halo-biphenyl derivatives and can be compared with 50·5° in 4-acetyl-2′-fluorobiphenyl (Young, Tollin & Sutherland, 1968) and 51·3° in 2′-iodo-4-biphenylcarboxylic acid (Sutherland, 1970). The axis of the molecule deviates from collinearity. Not only is there a rotation φ_1 about the C(1)–C(7) bond but also φ_2, the angle of rotation of the ring C(1)–C(6) about an axis in its plane through C(1) perpendicular to C(1)–C(7) is 0·7 (6)° and $\varphi_3 = 1·6$ (6)°, the corresponding angle of rotation for ring C(7)–C(12); there is a corresponding tilt, φ_5, of the nitro group about C(4) of 0·9 (5)°.

The shortest intermolecular contacts are 3·260 (10) Å between C(5) and N(1), 3·310 (8) Å between N(2) and O(1), 3·413 (10) Å between N(2) and O(2) and 3·381 (8) Å between C(6) and O(1), where N(1), O(1) and O(2) are at $1-x, -y, 1-z$ and 3·402 (10) Å between C(2) and C(2) at $1-x, 1-y, 1-z$.

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