Ring D is best described as having a twist conformation with the approximate C_2 axis through C(16). Puckering parameters for this ring are: $Q = 0.50$ Å, $\varphi = 92°$.

The molecular packing is shown in Fig. 5. Although the position of H(O3) could not be determined, it is most probable that the short O(3)–O(2^i) contact (2.74 Å) [(i) $x - \frac{1}{2}, \frac{1}{2} - y, 2 - z$] really represents a hydrogen bond. Only two other intermolecular distances shorter than 3.4 Å are observed. These are C(15)–O(4^{ii}) = 3.30 Å [(ii) $x + \frac{1}{2}, \frac{1}{2} - y, 2 - z$] and C(19)–O(4^{iii}) = 3.35 Å [(iii) $2 - x, y - \frac{1}{2}, 1\frac{1}{2} - z$].

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2e-(4-Nitrophenoxy)-trans-1-oxadecalin

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Abstract. $C_{15}H_{19}NO_4$, $M_r = 277.32$, monoclinic, $P2_1/c$, $a = 11.360$ (3), $b = 5.369$ (3), $c = 22.880$ (6) Å, $\beta = 100.05$ (2)°, $U = 1374$ Å^3, $Z = 4$, $D_x = 1.340$ Mg m^{-3}, μ(Mo $K\alpha$) = 0.06 mm^{-1}. The structure was refined to $R = 0.057$ for 1766 reflexions. The C–O lengths of the acetal group do not differ significantly either from each other, or from the corresponding equatorial phenoxy compound.

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Introduction. Our examination of the effects of ground-state structure on the reactivity of acetals (Jones, Kennard, Kirby & Osborne, 1978; Jones, Kennard, Kirby, Osborne & Malik, 1978) has revealed significant differences in the bond lengths and angles of the axial and equatorial isomers of 2-phenoxy-trans-1-oxadecalin [(I), $R = $ Ph] (Jones, Kennard, Chandrasekhar & Kirby, 1978a,b). In the axial isomer the exocyclic C–OR bond is longer than the endocyclic C–O(2) by 0.03 Å, though the lengths of these bonds in the equatorial isomer are not significantly different. These differences [which are in the opposite direction to

those of a similar magnitude observed for simple sugars such as glucose, where the exocyclic C—OH is the shorter in both axial and equatorial derivatives (Berman, Chu & Jeffrey, 1967)] presumably arise because the O atom of the phenoxy group is more electronegative than that of the pyranose ring.
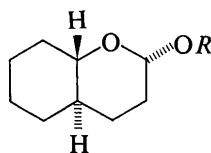
(I)

We are therefore extending this work to compounds with more electronegative aryloxy groups, and report here the structure of the equatorial derivative [(I), $R = p\text{-}C_6H_4NO_2$].

Flat colourless prisms elongated along **b** were obtained from dichloromethane/petroleum spirit. Since the compound is slowly hydrolysed by moisture, crystals were sealed in glass capillaries. A crystal 0·8 × 0·35 × 0·1 mm, mounted about **b**, was used to collect intensities at 280 K on a Stoe STADI-2 diffractometer (monochromated Mo $K\alpha$ radiation). 2300 reflexions were measured (layers 0–6); after application of Lp corrections, averaging equivalent reflexions gave 1771 unique reflexions with $F > 4\sigma(F)$. Systematic absences $h0l$, l odd and $0k0$, k odd indicated space group $P2_1/c$. Cell dimensions were obtained by least squares from ω values for 313 $h0l$ and 186 $hk0$ reflexions (the latter from the same crystal remounted about **c**).

The structure was solved with the program $XCSD$, which incorporates a pseudotangent refinement to select the starting set (Roberts, Pettersen, Sheldrick, Isaacs & Kennard, 1973) and the negative quartet test NQEST (DeTitta, Edmonds, Langs & Hauptman, 1975). The best E map showed all the non-H atoms.

Isotropic refinement proceeded to $R = 0\cdot13$ and anisotropic to $R = 0\cdot11$. At this stage a difference synthesis showed all the H atoms. In the final stages of refinement C—H distances were fixed at 1·08 Å and H—C—H angles at 109·5°, an overall isotropic temperature factor for H atoms was employed, and five low-angle reflexions with $F_o \ll F_c$ were omitted. Convergence was achieved at $R' = \sum w^{1/2}\Delta/\sum w^{1/2}|F_o| = 0\cdot063$, and $R = 0\cdot057$; the weighting scheme was $w = 1/[\sigma^2(F) + 0\cdot001\,F^2]$.

A final difference synthesis showed no peaks >0·24 e Å^{-3}. Final atomic coordinates are given in Table 1,

Table 1. *Atom coordinates* ($\times 10^4$)

The overall isotropic temperature factor for H atoms is 0·056 (2) Å^2.

	x	y	z
O(1)	3185 (1)	39 (3)	489 (1)
C(2)	1954 (2)	−27 (5)	518 (1)
C(3)	1754 (2)	−444 (5)	1143 (1)
C(4)	2394 (2)	1604 (6)	1546 (1)
C(5)	4333 (3)	4084 (6)	1815 (1)
C(6)	5604 (3)	4358 (6)	1698 (1)
C(7)	5630 (3)	4584 (6)	1037 (1)
C(8)	5014 (2)	2373 (6)	694 (1)
C(9)	3746 (2)	2172 (5)	811 (1)
C(10)	3691 (2)	1883 (5)	1468 (1)
C(11)	1415 (2)	−1964 (5)	−437 (1)
C(12)	795 (2)	−3907 (5)	−756 (1)
C(13)	724 (2)	−4021 (5)	−1368 (1)
C(14)	1275 (2)	−2159 (5)	−1641 (1)
C(15)	1867 (2)	−205 (5)	−1335 (1)
C(16)	1934 (2)	−82 (5)	−723 (1)
O(10)	1452 (2)	−2079 (3)	166 (1)
N(1)	1263 (2)	−2335 (5)	−2282 (1)
O(11)	670 (2)	−3943 (5)	−2562 (1)
O(12)	1857 (2)	−825 (5)	−2507 (1)
H(21)	1549	1726	363
H(31)	808	−386	1154
H(32)	2108	−2241	1297
H(41)	2369	1139	2003
H(42)	1936	3351	1436
H(51)	4361	3778	2284
H(52)	3844	5774	1681
H(61)	6116	2743	1871
H(62)	5999	6009	1921
H(71)	5177	6276	871
H(72)	6548	4656	972
H(81)	5496	685	838
H(82)	4999	2639	225
H(91)	3285	3879	664
H(101)	4150	215	1646
H(121)	369	−5318	−529
H(131)	253	−5520	−1624
H(151)	2275	1221	−1566
H(161)	2382	1456	−473

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

C(2)—O(1)	1·412 (4)	C(2)—C(3)	1·505 (5)
C(2)—O(10)	1·424 (4)	C(3)—C(4)	1·534 (6)
C(4)—C(10)	1·522 (6)	C(5)—C(6)	1·521 (6)
C(5)—C(10)	1·535 (6)	C(6)—C(7)	1·523 (6)
C(7)—C(8)	1·523 (6)	C(8)—C(9)	1·514 (6)
C(9)—O(1)	1·448 (4)	C(9)—C(10)	1·523 (5)
C(11)—C(12)	1·392 (4)	C(11)—C(16)	1·389 (5)
C(11)—O(10)	1·374 (4)	C(12)—C(13)	1·390 (4)
C(13)—C(14)	1·384 (5)	C(14)—C(15)	1·371 (4)
C(14)—N(1)	1·468 (4)	C(15)—C(16)	1·390 (4)
N(1)—O(11)	1·208 (4)	N(1)—O(12)	1·224 (4)

C(2)—O(1)—C(9)	110·3 (3)	O(1)—C(2)—C(3)	111·3 (3)
O(1)—C(2)—O(10)	107·2 (3)	O(10)—C(2)—O(10)	108·1 (3)
C(2)—C(3)—C(4)	109·3 (3)	C(3)—C(4)—C(10)	111·5 (3)
C(6)—C(5)—C(10)	111·3 (3)	C(5)—C(6)—C(7)	111·4 (3)
C(6)—C(7)—C(8)	111·3 (4)	C(7)—C(8)—C(9)	109·3 (3)
O(1)—C(9)—C(8)	108·3 (3)	O(1)—C(9)—C(10)	109·4 (3)
C(8)—C(9)—C(10)	112·7 (3)	C(4)—C(10)—C(5)	113·4 (3)
C(4)—C(10)—C(9)	109·5 (3)	C(5)—C(10)—C(9)	109·5 (3)
C(12)—C(11)—C(16)	121·1 (3)	C(12)—C(11)—O(10)	114·6 (3)
C(16)—C(11)—O(10)	124·3 (3)	C(11)—C(12)—C(13)	119·8 (3)
C(12)—C(13)—C(14)	118·1 (3)	C(13)—C(14)—C(15)	122·9 (3)
C(13)—C(14)—N(1)	118·5 (3)	C(15)—C(14)—N(1)	118·6 (3)
C(14)—C(15)—C(16)	119·1 (3)	C(11)—C(16)—C(15)	119·1 (3)
C(2)—O(10)—C(11)	118·2 (3)	C(14)—N(1)—O(11)	118·9 (3)
C(14)—N(1)—O(12)	117·9 (3)	O(11)—N(1)—O(12)	123·2 (3)

Table 3. *Selected torsion angles* (°)

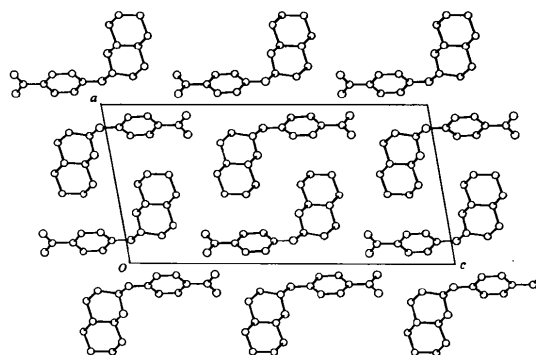The sign convention is as defined by Klyne & Prelog (1960).

C(9)—O(1)—C(2)—C(3)	−65·2 (3)	C(10)—C(5)—C(6)—C(7)	55·1 (4)	O(10)—C(11)—C(12)—C(13)	−178·3 (3)
C(9)—O(1)—C(2)—O(10)	176·8 (3)	C(6)—C(5)—C(10)—C(4)	−177·2 (3)	O(10)—C(11)—C(16)—C(15)	178·1 (3)
C(2)—O(1)—C(9)—C(8)	−172·0 (3)	C(6)—C(5)—C(10)—C(9)	−54·6 (4)	C(12)—C(11)—O(10)—C(2)	−173·2 (3)
C(2)—O(1)—C(9)—C(10)	64·9 (3)	C(5)—C(6)—C(7)—C(8)	−56·2 (4)	C(16)—C(11)—O(10)—C(2)	6·2 (4)
O(1)—C(2)—C(3)—C(4)	57·0 (4)	C(6)—C(7)—C(8)—C(9)	56·6 (4)	C(12)—C(13)—C(14)—N(1)	176·7 (3)
O(10)—C(2)—C(3)—C(4)	174·4 (3)	C(7)—C(8)—C(9)—O(1)	−179·1 (3)	N(1)—C(14)—C(15)—C(16)	−176·9 (3)
O(1)—C(2)—O(10)—C(11)	−66·9 (3)	C(7)—C(8)—C(9)—C(10)	−58·0 (4)	C(13)—C(14)—N(1)—O(11)	7·7 (5)
C(3)—C(2)—O(10)—C(11)	173·0 (3)	O(1)—C(9)—C(10)—C(4)	−57·5 (4)	C(13)—C(14)—N(1)—O(12)	−172·6 (3)
C(2)—C(3)—C(4)—C(10)	−50·6 (4)	O(1)—C(9)—C(10)—C(5)	177·5 (3)	C(15)—C(14)—N(1)—O(11)	−174·5 (3)
C(3)—C(4)—C(10)—C(5)	174·2 (3)	C(8)—C(9)—C(10)—C(4)	−178·1 (3)	C(15)—C(14)—N(1)—O(12)	5·2 (5)
C(3)—C(4)—C(10)—C(9)	51·6 (4)	C(8)—C(9)—C(10)—C(5)	57·0 (4)		
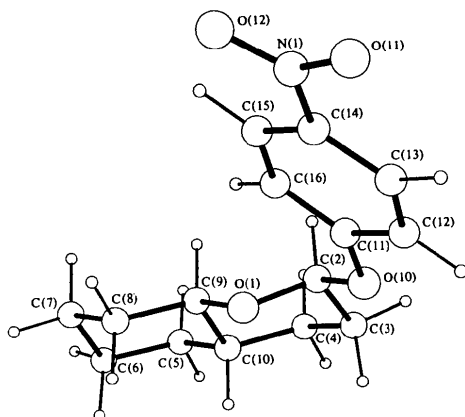
Fig. 1. The title compound showing the atom numbering. H atoms are numbered such that H(*mn*) is the *n*th H atom on C(*m*).

Fig. 2. Packing diagram projected down **b**. H atoms are omitted for clarity.

bond lengths and angles and torsion angles in Tables 2 and 3.* Diagrams of the structure are given in Figs. 1 and 2.

Discussion. The introduction of the 4-nitro group has had little effect on the bond lengths and angles about the acetal centre of (I). The angle O(1)—C(2)—O(10) is unchanged at 107·2° (Jones *et al.*, 1978b) and is consistent with the *trans,gauche* conformation adopted by both compounds (Gorenstein & Kar, 1977). The two C—O lengths are not significantly different [C(2)—O(1) = 1·412 (4), C(2)—O(10) = 1·424 (4) Å] either from each other, or from the corresponding lengths in the equatorial phenoxy compound [1·411 (3) and 1·415 (3) Å respectively; Jones *et al.*, 1978b]. Evidently, the transmission of electronic effects between the two O atoms of the acetal depends on the conformation about the acetal centre, and is minimal for the equatorial isomers in this series. This conclusion should be strengthened when data for the axial 4-nitrophenoxy compound become available.

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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 33939 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Short non-bonded contacts (<3·13 Å) are: O(11)··· N(1)(−x, −½ + y, −½ − z) 2·83, O(12)···O(11)(−x, ½ + y, −½ − z) 3·07, O(11)···O(11)(−x, ½ + y, −½ − z) 3·12 Å.

The figures were drawn with *PLUTO* written by Dr W. D. S. Motherwell; all other crystallographic programs were written by Dr G. M. Sheldrick. We thank the MRC for financial support.

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