

Table 1. Fractional atomic coordinates ( $\times 10^4$  for O, N, C;  $\times 10^3$  for H) and equivalent isotropic thermal parameters ( $\text{\AA}^2 \times 10^3$ )

	x	y	z	$U_{iso}/U_{eq}$
O	2539 (2)	1193 (3)	4605 (1)	65 (1)*
N	3712 (2)	1962 (3)	4659 (1)	50 (1)*
C1	4147 (3)	2879 (4)	4026 (1)	64 (2)*
C2	4478 (3)	1985 (4)	5218 (1)	49 (1)*
C3	4168 (3)	1246 (3)	5888 (1)	46 (1)*
C4	3035 (3)	220 (3)	6036 (1)	52 (1)*
C5	2812 (3)	-361 (4)	6710 (1)	61 (2)*
C6	3716 (4)	47 (4)	7245 (1)	65 (2)*
C7	4850 (3)	1027 (4)	7104 (1)	64 (2)*
C8	5093 (3)	1612 (4)	6436 (1)	54 (2)*
H1a	344 (3)	385 (4)	394 (1)	53 (9)
H1b	403 (3)	216 (4)	365 (1)	41 (8)
H1c	506 (4)	334 (5)	405 (2)	78 (12)
H2	530 (3)	261 (3)	516 (1)	20 (7)
H4	245 (3)	-6 (3)	567 (1)	23 (7)
H5	209 (3)	-115 (4)	682 (1)	39 (9)
H6	354 (3)	-35 (3)	772 (1)	36 (8)
H7	551 (3)	129 (4)	747 (2)	56 (9)
H8	588 (3)	234 (3)	633 (1)	27 (7)

\*  $U_{eq}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

Table 2. Intramolecular distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) with e.s.d.'s in parentheses

O—N	1.293 (3)	N—C1	1.473 (4)
N—C2	1.298 (3)	C2—C3	1.438 (4)
C3—C4	1.395 (4)	C3—C8	1.406 (4)
C4—C5	1.383 (4)	C5—C6	1.383 (4)
C6—C7	1.373 (5)	C7—C8	1.378 (4)
O—N—C1	114.8 (2)	O—N—C2	124.9 (2)
C1—N—C2	120.3 (2)	N—C2—C3	127.2 (2)
C2—C3—C4	125.7 (2)	C2—C3—C8	116.2 (2)
C4—C3—C8	118.1 (2)	C3—C4—C5	120.4 (2)
C4—C5—C6	120.6 (3)	C5—C6—C7	119.6 (3)
C6—C7—C8	120.7 (3)	C3—C8—C7	120.5 (3)

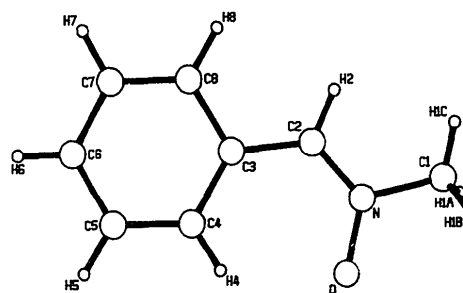


Fig. 1. Molecular structure and numbering scheme for PhCH=N(Me)O.

Taylor, 1985; Pritchard, Banks, DuBoisson & Tipping, 1991).

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## Mesogenic 4'-(4-Hydroxy-1-butoxy)biphenyl-4-carbonitrile and Non-Mesogenic 4-(4'-Cyano-4-biphenyloxy)-1-butyl Acrylate

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**Abstract.** (A)  $C_{17}H_{17}NO_2$ ,  $M_r = 267.3$ , triclinic,  $P\bar{1}$ ,  $a = 14.418$  (6),  $b = 9.236$  (4),  $c = 5.651$  (3)  $\text{\AA}$ ,  $\alpha = 89.91$  (2),  $\beta = 85.37$  (2),  $\gamma = 72.93$  (2) $^\circ$ ,  $V = 716.8$   $\text{\AA}^3$ ,

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$Z = 2$ ,  $D_x = 1.238$   $\text{g cm}^{-3}$ ,  $\lambda(\text{Mo } K\alpha) = 0.71069$   $\text{\AA}$ ,  $\mu = 0.46$   $\text{cm}^{-1}$ ,  $F(000) = 284$ ,  $T = 295$  K, final  $R = 0.0820$  for 1942 unique reflections with  $F_o > 3\sigma(F_o)$ . (B)  $C_{20}H_{19}NO_3$ ,  $M_r = 321.4$ , triclinic,  $P\bar{1}$ ,  $a = 12.978$  (4),  $b = 9.941$  (3),  $c = 6.971$  (2)  $\text{\AA}$ ,  $\alpha = 95.81$  (1),  $\beta = 100.63$  (1),  $\gamma = 102.62$  (1) $^\circ$ ,  $V = 853.1$   $\text{\AA}^3$ ,  $Z = 2$ ,  $D_x = 1.251$   $\text{g cm}^{-3}$ ,  $\lambda(\text{Mo } K\alpha) = 0.71069$   $\text{\AA}$ ,  $\mu = 0.48$   $\text{cm}^{-1}$ ,  $F(000) = 340$ ,  $T = 297$  K,

final  $R = 0.0472$  for 2768 unique reflections with  $F_o > 2\sigma(F_o)$ . Both compounds NC— $\phi''$ — $\phi'$ —O—C<sub>4</sub>H<sub>9</sub>—O—R [ $R = \text{H}$  (A),  $R = \text{C}(\text{O})\text{—CHCH}_2$  (B)] crystallize in their long extended conformation. Dihedral angles in (A):  $\phi''[\text{C}(2)\text{—C}(7)]/\phi'[\text{C}8\text{—C}(13)] = -22.3$ ,  $\phi'/\text{C}_4[\text{C}(14)\text{—C}(17)] = 10.6$ ; in (B):  $\phi''/\phi' = -39.6$ ,  $\phi'/\text{C}_4 = 58.9$ ,  $\text{C}_4/\text{OC}(\text{O})\text{C}=\text{C} = 22.0^\circ$ . Hydrogen bonding between the alcohol and the cyano end groups  $[\text{O}(x+1, y-1, z+2)\cdots\text{N} = 2.890$  (5) Å] leads to crystal packing as chains along  $[1\bar{1}2]$  for (A). In (B) chains along  $[103]$  are formed. No evidence for intermolecular interactions such as phenyl–cyano or phenyl–phenyl contacts is found in either compound.

**Experimental.** Intensity data for (A) and (B) were collected on a Stoe-Stadi 4 diffractometer using graphite-monochromated Mo  $K\alpha$  radiation, scan mode  $\omega:2\theta = 1:1$  (Clegg, 1981). Both structures solved by direct methods (SHELXS90; Sheldrick, 1990) and refined with SHELX76 (Sheldrick, 1976). Weighting scheme  $w = k[\sigma(F_o)^2]^{-1}$ ,  $k$  determined by least squares. Scattering factors as stored in SHELX76.

(A). Colorless needles crystallized from an acetone–water solution. Standards recorded after each 1.5 h measuring time, decrease  $< 1\%$ . Lp correction applied, no absorption correction. H atoms in geometrically idealized positions (C—H = 0.96 Å) except the alcoholic H(O2) atom which was localized in a difference Fourier synthesis and fixed. Anisotropic temperature factors for atoms C, N, O, for H atoms fixed  $U_{\text{iso}}(\text{H}) = 0.050 \text{ \AA}^2$ .

(B). Flat colorless prisms were obtained from the reaction of (A) with acrylic acid (Quotschalla, 1989) and crystallized from an acetone–water solution. Standards recorded every hour during measuring time showed no significant intensity variation. Lp correction applied, no absorption correction. All H atoms localized in a difference Fourier map and refined. Anisotropic temperature factors for atoms C, N, O, for H atoms fixed  $U_{\text{iso}}(\text{H}) = 0.050 \text{ \AA}^2$ .

Other experimental details are summarized in Table 1. Atomic parameters and selected bond lengths and angles are given in Tables 2\* and 3. The molecules with atomic labeling schemes and packing diagrams (PLUTO; Motherwell & Clegg, 1978) are presented in Figs. 1 and 2. Best planes were calculated with a locally written program (PLAN; Costines, Foitzik & Gehring, 1984).

\* Lists of structure factors, anisotropic thermal parameters and H-atom positional parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54226 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Experimental details

	(A)	(B)
Crystal dimensions (mm)	1.0 × 0.3 × 0.2	0.7 × 0.3 × 0.2
Unit cell		
Number of reflections	58	52
2 $\theta$ range (°)	35.9 ≤ 2 $\theta$ ≤ 40.6	14.5 ≤ 2 $\theta$ ≤ 45.2
Standards	121, 402, 220	203, 310, 230
2 $\theta$ range (°)	3 < 2 $\theta$ < 50	3 < 2 $\theta$ < 50
$hkl$ range	-17 ≤ $h$ ≤ 17 -10 ≤ $k$ ≤ 10 -6 ≤ $l$ ≤ 6	-15 ≤ $h$ ≤ 15, -11 ≤ $k$ ≤ 11 -8 ≤ $l$ ≤ 5
Reflections		
Total	5003	5500
Unique	2503	2898
Observed	1942 [ $F_o > 3\sigma(F_o)$ ]	2768 [ $F_o > 2\sigma(F_o)$ ]
$R_{\text{int}}$ (SHELX76)	0.0151	0.0167
Parameters refined	182	275
$R, wR$	0.0820, 0.0662	0.0472, 0.0503
Mean, max. shift/e.s.d.	0.02, 0.06	0.02, 0.11
$\Delta\rho$ (e Å <sup>-3</sup> )	0.30, -0.23	0.18, -0.18

Table 2. Atomic positional parameters and equivalent isotropic thermal parameters with e.s.d.'s in parentheses for (A) and (B)

$$U_{\text{eq}} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j$$

	x	y	z	$U_{\text{eq}}$ (Å <sup>2</sup> )
(A)				
O(1)	0.0049 (2)	0.8169 (2)	0.2897 (4)	0.083 (2)
O(2)	-0.2999 (2)	0.9020 (3)	-0.4029 (5)	0.124 (3)
N(1)	0.5854 (2)	0.1640 (4)	1.3616 (6)	0.112 (3)
C(1)	0.5272 (3)	0.2347 (4)	1.2517 (6)	0.087 (3)
C(2)	0.4518 (2)	0.3214 (4)	1.1085 (6)	0.069 (3)
C(3)	0.3986 (2)	0.4677 (4)	1.1727 (6)	0.075 (3)
C(4)	0.3259 (2)	0.5468 (3)	1.0383 (5)	0.069 (3)
C(5)	0.3040 (2)	0.4832 (3)	0.8354 (5)	0.059 (3)
C(6)	0.3597 (2)	0.3359 (3)	0.7721 (6)	0.072 (3)
C(7)	0.4326 (2)	0.2553 (3)	0.9062 (6)	0.076 (3)
C(8)	0.2248 (2)	0.5680 (3)	0.6910 (5)	0.061 (3)
C(9)	0.1915 (2)	0.7247 (3)	0.6968 (6)	0.074 (3)
C(10)	0.1187 (2)	0.8031 (3)	0.5621 (6)	0.077 (3)
C(11)	0.0766 (2)	0.7267 (3)	0.4150 (6)	0.067 (3)
C(12)	0.1073 (2)	0.5719 (3)	0.4053 (6)	0.071 (3)
C(13)	0.1812 (2)	0.4940 (3)	0.5419 (5)	0.068 (3)
C(14)	-0.0378 (2)	0.7490 (3)	0.1216 (6)	0.075 (3)
C(15)	-0.1192 (2)	0.8761 (3)	0.0303 (6)	0.085 (3)
C(16)	-0.1728 (2)	0.8283 (3)	-0.1486 (6)	0.082 (3)
C(17)	-0.2585 (2)	0.9538 (3)	-0.2200 (6)	0.086 (3)
(B)				
O(1)	0.2957 (1)	0.2013 (1)	0.2206 (2)	0.057 (1)
O(2)	0.4947 (1)	0.2889 (1)	0.9500 (2)	0.058 (1)
O(3)	0.5824 (1)	0.1795 (1)	1.1663 (2)	0.071 (1)
N(1)	-0.2248 (1)	0.3141 (2)	-1.1626 (2)	0.085 (1)
C(1)	-0.1708 (1)	0.3077 (2)	-1.0165 (3)	0.063 (1)
C(2)	-0.1037 (1)	0.2991 (2)	-0.8310 (2)	0.053 (1)
C(3)	0.0064 (1)	0.3553 (2)	-0.7905 (3)	0.066 (1)
C(4)	0.0697 (1)	0.3424 (2)	-0.6149 (3)	0.063 (1)
C(5)	0.0250 (1)	0.2732 (2)	-0.4758 (2)	0.048 (1)
C(6)	-0.0860 (1)	0.2193 (2)	-0.5180 (3)	0.060 (1)
C(7)	-0.1503 (1)	0.2317 (2)	-0.6930 (3)	0.061 (1)
C(8)	0.0933 (1)	0.2540 (2)	-0.2900 (2)	0.048 (1)
C(9)	0.1816 (1)	0.3587 (2)	-0.1858 (2)	0.050 (1)
C(10)	0.2462 (1)	0.3391 (2)	-0.0160 (2)	0.050 (1)
C(11)	0.2252 (1)	0.2128 (2)	0.0541 (2)	0.048 (1)
C(12)	0.1372 (1)	0.1076 (2)	-0.0455 (3)	0.059 (1)
C(13)	0.0725 (1)	0.1292 (2)	-0.2148 (2)	0.058 (1)
C(14)	0.2781 (2)	0.0703 (2)	0.2932 (3)	0.065 (1)
C(15)	0.3719 (2)	0.0727 (2)	0.4571 (3)	0.059 (1)
C(16)	0.3881 (2)	0.1832 (2)	0.6323 (3)	0.058 (1)
C(17)	0.4736 (2)	0.1699 (2)	0.7989 (3)	0.064 (1)
C(18)	0.5507 (1)	0.2807 (2)	1.1274 (2)	0.050 (1)
C(19)	0.5675 (1)	0.4084 (2)	1.2660 (3)	0.059 (1)
C(20)	0.6199 (2)	0.4249 (2)	1.4475 (3)	0.070 (1)

Table 3. Selected bond distances (Å) and angles (°) with *e.s.d.*'s in parentheses

N(1)—C(1)	1.130 (3)	1.140 (2)
C(1)—C(2)	1.452 (4)	1.442 (2)
C(5)—C(8)	1.486 (3)	1.483 (2)
O(1)—C(11)	1.370 (3)	1.370 (2)
O(1)—C(14)	1.413 (3)	1.432 (2)
C(14)—C(15)	1.520 (3)	1.502 (2)
C(15)—C(16)	1.464 (4)	1.509 (2)
C(16)—C(17)	1.507 (4)	1.489 (2)
O(2)—C(17)	1.386 (3)	1.444 (2)
O(2)—C(18)		1.334 (2)
O(3)—C(18)		1.204 (2)
C(18)—C(19)		1.466 (2)
C(19)—C(20)		1.297 (2)
O(2)⋯N(1)	2.890 (5)	
O(2)—H(O2)	0.99 (1)	
	(A)	(B)
Phenyl ring C(2) to C(7): mean C—C	1.382	1.382
Phenyl ring C(8) to C(13): mean C—C	1.378	1.384
Mean C—H distances:		
C <sub>arom</sub> —H	0.96*	0.95
C <sub>aliph</sub> —H	0.96*	0.97
C <sub>vinyl</sub> —H		0.94
	(A)	(B)
N(1)—C(1)—C(2)	178.3 (4)	179.3 (2)
C(1)—C(2)—C(3)	121.0 (3)	121.0 (2)
C(1)—C(2)—C(7)	119.4 (3)	119.4 (2)
C(5)—C(8)—C(9)	121.8 (3)	121.8 (1)
C(5)—C(8)—C(13)	121.5 (3)	120.9 (1)
C(11)—O(1)—C(14)	119.1 (2)	117.4 (1)
O(1)—C(14)—C(15)	106.1 (2)	109.0 (1)
C(14)—C(15)—C(16)	114.5 (3)	114.4 (1)
C(15)—C(16)—C(17)	113.3 (3)	111.9 (1)
C(16)—C(17)—O(2)	109.3 (3)	108.8 (1)
C(17)—O(2)—C(18)		117.1 (1)
O(2)—C(18)—O(3)		123.3 (2)
O(2)—C(18)—C(19)		111.7 (1)
O(3)—C(18)—C(19)		125.0 (1)
C(18)—C(19)—C(20)		122.9 (2)

Symmetry code: (i)  $x + 1, y - 1, z + 2$ .

\* Fixed.

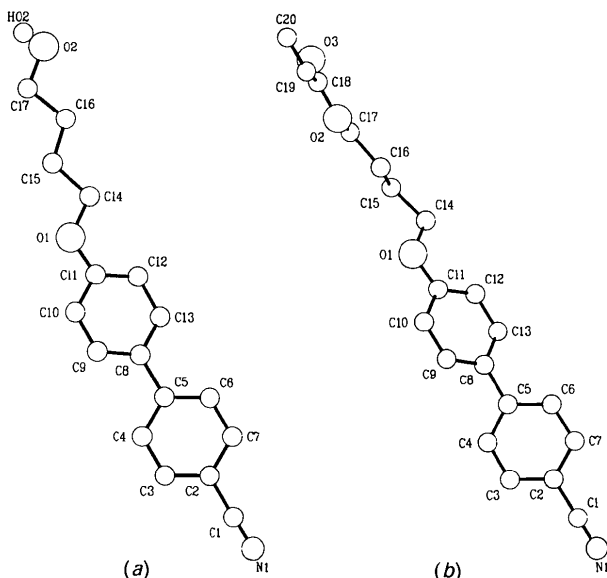
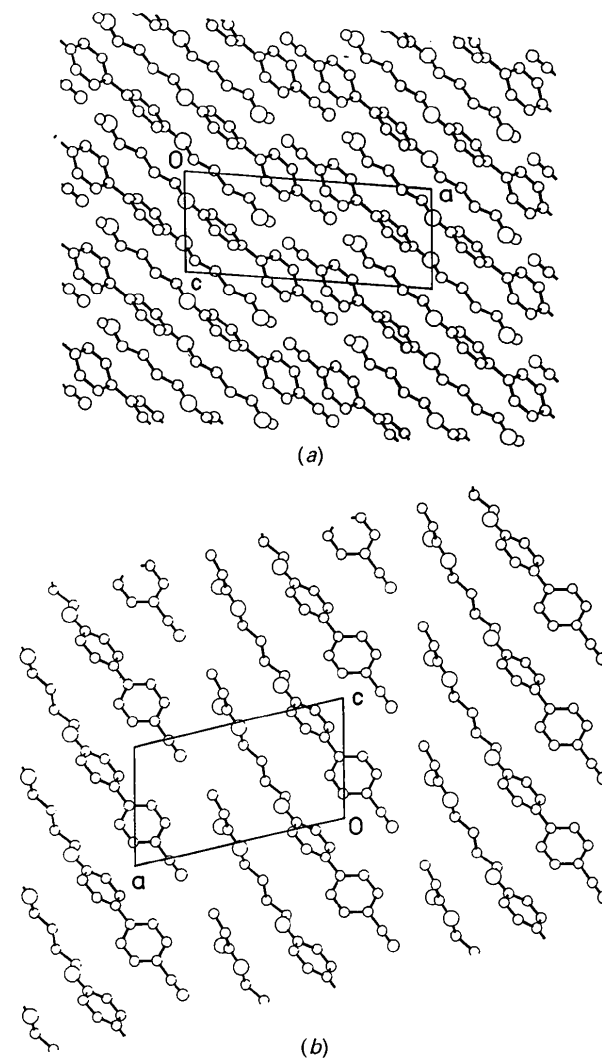


Fig. 1. Molecular structure of (a) (A) and (b) (B) projected on a plane defined by C(2), C(4), C(6).

**Related literature.** The mesogenic (A) and the non-mesogenic (B) are monomeric fragments of a liquid crystalline side-chain polymer (Portugall, Ringsdorf & Zentel, 1982; Shibaev, Kostromin & Platé, 1982). Dihedral angles in mesogenic biphenyls are studied by Haase, Paulus & Müller (1983), Walz, Paulus & Haase (1987) and Walz, Nepveu & Haase (1987). The question of whether solid phases of mesomorphic compounds can be regarded as precursors for the structure in the mesophase is the subject of present work by Haase, Walz & Loub (1991).

We thank Dr Dorsch, E. Merck Company, Darmstadt, for providing the mesogen (A). Financial support by the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

Fig. 2. Crystal packing of (a) (A) viewed along [010] and (b) (B) viewed along [010],  $0 < y < 0.5$ .

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## Structure of (2'R\*,5S\*)-(±)-5-(Tetrahydro-2'H-pyran-2'-yl)-2(5H)-furanone

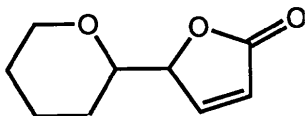
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**Abstract.** C<sub>9</sub>H<sub>12</sub>O<sub>3</sub>,  $M_r = 168.2$ , triclinic,  $P\bar{1}$ ,  $a = 5.5385(6)$ ,  $b = 8.543(1)$ ,  $c = 10.373(1)$  Å,  $\alpha = 113.329(9)^\circ$ ,  $\beta = 100.78(1)^\circ$ ,  $\gamma = 99.82(1)^\circ$ ,  $V = 426.2(2)$  Å<sup>3</sup>,  $D_x = 1.31$  g cm<sup>-3</sup>,  $Z = 2$ , Cu  $K\alpha$  ( $\lambda = 1.54178$  Å, graphite monochromator),  $\mu = 8.2$  cm<sup>-1</sup>,  $F(000) = 180$ ,  $T = 293$  K. Final  $R = 0.036$ ,  $wR = 0.081$  for 1559 reflections with  $I > 3\sigma(I)$ . The relative configurations at the two chiral centers are (*S*,*R*). The dihedral angle between the five- and six-membered rings (O1—C4—C5—O3) is  $69.9(1)^\circ$ . The tetrahydropyran is in a chair conformation with the furanone ring equatorial.

**Experimental.** Colorless crystals from pentane,  $0.3 \times 0.4 \times 0.5$  mm block-like specimen; Enraf–Nonius CAD-4 diffractometer; cell parameters and crystal orientation from 25 automatically centered reflections in the range  $8.9 < \theta < 48.8^\circ$ ;  $2\theta$ – $\theta$  scans over



$\Delta\theta$  range of  $1.5(1.0 + 0.14\tan\theta)^\circ$ ; variable  $\theta$  scan speed of  $8.24$ – $1.18^\circ$  min<sup>-1</sup>; each scan recorded in 96 steps with two outermost 16 step intensity blocks used for background determination; diffractometer controlled with Digital Equipment Corporation MicroVAX II computer and standard Enraf–Nonius programs (version 5.0); seven standard reflections monitored at 1 h intervals of X-ray exposure,  $-9.7$

to  $-2.0\%$  intensity variation,  $-5.0\%$  average, correction applied;  $\psi$ -scan absorption correction with data from five reflections, transmission-factor range of  $0.973$ – $1.000$ , average of  $0.985$ ;  $4.8 < \theta < 70^\circ$ ,  $hkl$ 's selected to maintain diffractometer  $\chi$  angle within  $0$ – $90^\circ$  range; 1703 total data measured, 1624 unique data, 1559 data with  $I > 3\sigma(I)$ ,  $R_{\text{int}} = 0.0$  for nine twice-measured data. All crystallographic calculations performed with the *TEXSAN* (Molecular Structure Corporation, 1989) program system on DEC MicroVAX II or VAXStation II computers; structure solved with the *MITHRIL* (Gilmore, 1983) direct-methods program incorporated in *TEXSAN*. Full-matrix least-squares refinement,  $\sum[w(F_o - F_c)^2]$  minimized with  $w = 1/\sigma^2(F_o)$ , reflections with  $I < 3\sigma(I)$  excluded from refinement, correction for secondary isotropic extinction (Zachariasen, 1968) applied,  $g = 0.88(13) \times 10^{-4}$ ; C and O refined with anisotropic temperature factors; H atoms initially positioned from the C-atom framework and refined with individual isotropic temperature factors; 158 total variables; atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 155–175); minimum and maximum  $\Delta\rho$  of  $-0.13$  and  $0.19$  e Å<sup>-3</sup>; maximum  $\Delta/\sigma$  in final least-squares cycle of  $0.08$ ;  $R$ ,  $wR$  and  $S$  of  $0.036$ ,  $0.081$  and  $2.93$ . Atomic coordinates are listed in Table 1;\*

\* Lists of structure factors, anisotropic temperature factors, and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54296 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.