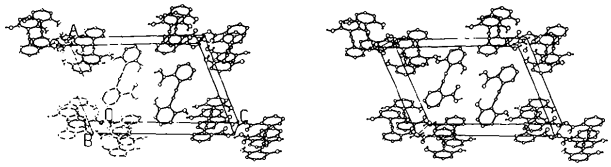

Fig. 2. Stereoview of the unit cell, viewed slightly oblique to the *b* axis with *c* horizontal.

angles are given in Table 2. The molecule is illustrated in Fig. 1. The unit cell is illustrated in Fig. 2.

Related literature. Structure of methyl 2-[(2,6-dimethoxyphenyl)ethynyl]benzoate: Huang, Evans, Fronczek & Gandour (1991). Structure of methyl 2-[(2,6-dimethoxyphenyl)ethynyl]-3-methoxybenzoate: Evans, Horn, Fronczek & Gandour (1990). Structure of diphenylacetylene: Mavridis & Moustakali-Mavridis (1977). Structure of bis(*m*-chlorophenyl)acetylene: Espiritu & White (1977). Structure of *p*-butyl-*p*′-methoxydiphenylacetylene: Cotrait (1977).

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Acta Cryst. (1992). C**48**, 765–767

3-(2,6-Dihydroxyphenyl)-1*H*-2-benzopyran-1-one

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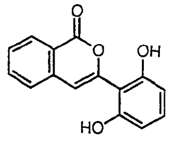
Abstract. $C_{15}H_{10}O_4$, $M_r = 254.2$, monoclinic, $P2_1$, $a = 5.9476$ (4), $b = 8.1253$ (10), $c = 12.0198$ (12) Å, $\beta = 100.938$ (7)°, $V = 570.3$ (2) Å^3, $Z = 2$, $D_x = 1.480$ g cm^{-3} at 297 K, λ(Cu $K\alpha$) = 1.54184 Å, $\mu = 8.56$ cm^{-1}, $F(000) = 264$, 1268 unique data, final $R = 0.035$ for 1113 reflections with $I > 3.0\sigma(I)$. Maximum deviations from planarity of the two aromatic rings are 0.008 (3) Å for the ring containing the two hydroxy substituents and 0.006 (4) Å for the aromatic ring of the benzopyran. The two rings form a dihedral angle of 113.3 (1)°. The C═C double bond distance is 1.330 (3) Å. Two distinct intermolecular hydrogen bonds are observed. One hydroxy group donates an intermolecular hydrogen bond to the carbonyl O atom of a second molecule, and also accepts a second intermolecular hydrogen bond from a hydroxy group of a third molecule. The former hydrogen bond has O···O distance 2.680 (3) Å and angle at H of 175 (4)°, while the latter has O···O distance 2.763 (3) Å and angle at H of 152 (3)°.

Experimental. The title compound was isolated as a side product of the demethylation of methyl 2-[(2,6-dimethoxyphenyl)ethynyl]benzoate using boron tribromide. Colorless plates of (1) were isolated by slow evaporation from methanol. Crystal size 0.02 × 0.25 × 0.30 mm, space group from systematic absences 0*k*0 with *k* odd, cell dimensions from setting angles of 25 reflections having $20 < \theta < 25°$. Data collection on Enraf–Nonius CAD-4 diffrac-



(1)

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* To whom correspondence should be addressed.

Table 1. *Coordinates and isotropic thermal parameters* (Å^2)

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
O1	−0.3668 (3)	1	−0.0899 (1)	3.07 (3)
O2	0.2718 (3)	0.6551 (3)	−0.1183 (1)	3.57 (4)
O3	−0.2880 (3)	0.6597 (3)	0.2221 (2)	3.80 (4)
O4	−0.1565 (3)	0.7476 (3)	0.0743 (1)	2.67 (3)
C1	−0.2392 (4)	0.9194 (3)	−0.1561 (2)	2.52 (5)
C2	−0.2882 (5)	0.9294 (4)	−0.2726 (2)	3.11 (5)
C3	−0.1455 (5)	0.8511 (4)	−0.3346 (2)	3.60 (6)
C4	0.0404 (5)	0.7613 (4)	−0.2819 (2)	3.36 (5)
C5	0.0886 (4)	0.7501 (4)	−0.1650 (2)	2.74 (5)
C6	−0.0488 (4)	0.8305 (4)	−0.0993 (2)	2.42 (4)
C7	0.0070 (4)	0.8299 (3)	0.0257 (2)	2.31 (4)
C8	0.1890 (4)	0.8990 (4)	0.0901 (2)	2.70 (5)
C9	0.2183 (4)	0.8962 (3)	0.2118 (2)	2.52 (5)
C10	0.4031 (4)	0.9724 (4)	0.2829 (2)	3.25 (6)
C11	0.4167 (5)	0.9697 (5)	0.3982 (3)	3.95 (6)
C12	0.2516 (6)	0.8896 (5)	0.4462 (2)	4.14 (7)
C13	0.0695 (5)	0.8136 (4)	0.3782 (2)	3.48 (6)
C14	0.0525 (4)	0.8171 (3)	0.2616 (2)	2.52 (4)
C15	−0.1395 (4)	0.7365 (4)	0.1883 (2)	2.67 (5)

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

O1—C1	1.367 (3)	C6—C7	1.475 (3)
O2—C5	1.366 (3)	C7—C8	1.330 (3)
O3—C15	1.213 (3)	C8—C9	1.440 (3)
O4—C7	1.396 (3)	C9—C10	1.402 (3)
O4—C15	1.358 (3)	C9—C14	1.403 (4)
C1—C2	1.378 (3)	C10—C11	1.373 (4)
C1—C6	1.406 (3)	C11—C12	1.391 (5)
C2—C3	1.386 (4)	C12—C13	1.374 (4)
C3—C4	1.375 (4)	C13—C14	1.386 (4)
C4—C5	1.382 (3)	C14—C15	1.459 (3)
C5—C6	1.401 (4)		
C7—O4—C15	122.0 (2)	C6—C7—C8	126.3 (2)
O1—C1—C2	122.0 (2)	C7—C8—C9	120.8 (2)
O1—C1—C6	116.6 (2)	C8—C9—C10	122.8 (2)
C2—C1—C6	121.3 (2)	C8—C9—C14	118.8 (2)
C1—C2—C3	119.1 (2)	C10—C9—C14	118.4 (2)
C2—C3—C4	121.1 (2)	C9—C10—C11	119.9 (3)
C3—C4—C5	119.8 (3)	C10—C11—C12	121.0 (3)
O2—C5—C4	116.8 (2)	C11—C12—C13	120.1 (3)
O2—C5—C6	122.4 (2)	C12—C13—C14	119.4 (3)
C4—C5—C6	120.8 (2)	C9—C14—C13	121.2 (2)
C1—C6—C5	117.9 (2)	C9—C14—C15	118.7 (2)
C1—C6—C7	120.1 (2)	C13—C14—C15	120.0 (2)
C5—C6—C7	122.0 (2)	O3—C15—O4	116.9 (2)
O4—C7—C6	112.8 (2)	O3—C15—C14	124.4 (2)
O4—C7—C8	120.9 (2)	O4—C15—C14	118.7 (2)

tometer, Cu $K\alpha$ radiation, graphite monochromator, ω–2θ scans designed for $I = 25\sigma(I)$, subject to maximum scan time = 120 s, scan rates varied 0.63–3.30° min^{-1}. One quadrant of data having $2 < \theta < 75°$, $0 \le h \le 7$, $0 \le k \le 10$, $-15 \le l \le 15$ measured. Data corrected for background, Lorentz and polarization effects. The standard reflections 200, 020, 006 decreased in intensity by 5.3% during data collection, and a linear correction was applied. Absorption corrections were based on ψ scans, with relative transmission coefficients ranging from 0.9264 to 0.9979. 1450 total data were collected, and redundant $0kl$ and $0k\bar{l}$ data merged, $R_{int} = 0.016$, to yield 1268 unique data, 1113 observed with $I > 3\sigma(I)$. Structure solved by direct methods using *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982), refined by full-matrix least squares based on F with weights $w = 4F_o^2[\sigma^2(I) + (0.02F_o^2)^2]^{-1}$ using *Enraf–Nonius SDP/VAX* (Frenz & Okaya, 1980), scattering factors of Cromer & Waber (1974), anomalous coefficients of Cromer (1974). Non-H atoms refined anisotropically; H atoms located from difference maps and refined isotropically. Final $R = 0.035$ (0.043 for all data), $wR = 0.043$, $S = 1.900$ for 212 variables. Maximum shift $< 0.01\sigma$ in the final cycle, maximum residual density 0.22 e Å^{-3}, minimum −0.14 e Å^{-3}, extinction coefficient (Larson, 1969) $g = 6.5\,(7) \times 10^{-6}$, where the correction factor $(1 + gI_c)^{-1}$ was applied to F_c, maximum correction 18.6% for the 120 reflection.

Coordinates* and equivalent isotropic thermal parameters are given in Table 1; bond distances and angles are given in Table 2. The molecule is illustrated in Fig. 1. The unit cell is illustrated in Fig. 2.

Related literature. Structure of methyl 2-[(2,6-dimethoxyphenyl)ethynyl]benzoate: Huang, Evans,

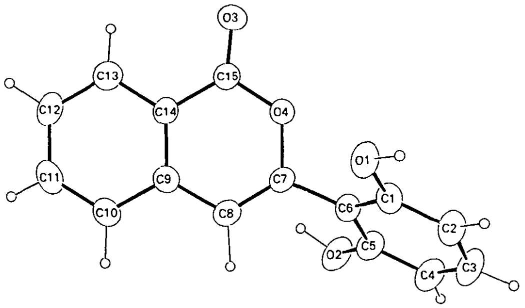

Fig. 1. *ORTEP* (Johnson, 1965) drawing of the title compound, with thermal ellipsoids drawn at the 40% probability level, and H atoms represented by circles of arbitrary radius.

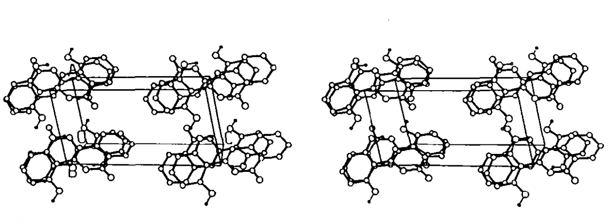

Fig. 2. Stereoview of unit cell, viewed slightly oblique to the b axis, with c horizontal

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* Lists of H-atom coordinates, bond distances and angles involving H atoms, torsion angles, anisotropic thermal parameters, least-squares-planes data, and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54644 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST0545]

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Acta Cryst. (1992). C**48**, 767–768

Structure of 3-Iodo-2,5-diphenyltellurophene, $C_{16}H_{11}ITe$

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Abstract. $C_{16}H_{11}ITe$, $M_r = 457.74$, orthorhombic, $Pbca$, $a = 8.588$ (1), $b = 24.280$ (3), $c = 13.992$ (2) Å, $V = 2918$ (1) Å^3, $Z = 8$, $D_x = 2.084$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 41.18$ mm^{-1}, $F(000) = 1696$, $T = 298$ K, $R = 0.043$ for 1617 observed reflections. The heterocyclic ring is essentially planar making dihedral angles of 126.0 (2) and 29.2 (5)° with the phenyl rings. Distances and angle around the Te atom are: Te—C 2.077 (9), 2.070 (9) Å and C—Te—C 82.7 (4)°.

Experimental. The data collection and refinement parameters are summarized in Table 1. The structure was solved using standard direct methods and difference Fourier techniques. In the final cycles of full-matrix least-squares refinement on F all non-H atoms were treated anisotropically; the H atoms were included, as fixed contributors, at positions found in a difference Fourier synthesis, all with a common isotropic temperature factor that refined to $U = 0.07$ (1) Å^2. Data were corrected for Lp and absorption, with maximum and minimum transmission factors of 1.59 and 0.84 (Walker & Stuart, 1983). Scattering factors for non-H atoms were taken from Cromer & Mann (1968) with corrections for anomalous dispersion taken from Cromer & Liberman (1970); for H atoms from Stewart, Davidson & Simpson (1965). Programs used: *SHELX*76 (Sheldrick, 1976) and *ORTEP* (Johnson, 1965). Most of the calculations were performed on a VAX 4620 computer of the Instituto de Física e Química de São Carlos.

Atomic coordinates are listed in Table 2,* bond lengths and bond angles are listed in Table 3. Fig. 1

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* Lists of H-atom positions, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54698 (20 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI0110]