

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

O(1)—C(2)	1.373 (2)	C(6)—C(15)	1.507 (2)
O(1)—C(9)	1.378 (2)	C(7)—C(8)	1.402 (2)
C(2)—C(3)	1.446 (2)	C(7)—N(12)	1.356 (2)
C(2)—O(11)	1.204 (2)	C(8)—C(9)	1.379 (2)
C(3)—C(4)	1.350 (2)	C(9)—C(10)	1.398 (2)
C(4)—C(10)	1.430 (2)	N(12)—C(13)	1.452 (2)
C(4)—C(16)	1.509 (2)	C(13)—C(14)	1.504 (3)
C(5)—C(6)	1.371 (2)	C(16)—F(17)	1.323 (2)
C(5)—C(10)	1.416 (2)	C(16)—F(18)	1.333 (2)
C(6)—C(7)	1.432 (2)	C(16)—F(19)	1.333 (2)
C(2)—O(1)—C(9)	122.3 (2)	O(1)—C(9)—C(8)	115.7 (2)
O(1)—C(2)—O(11)	117.1 (2)	C(8)—C(9)—C(10)	122.8 (2)
O(1)—C(2)—C(3)	116.8 (2)	O(1)—C(9)—C(10)	121.5 (2)
C(3)—C(2)—O(11)	126.1 (2)	C(5)—C(10)—C(9)	116.4 (2)
C(3)—C(4)—C(16)	118.6 (2)	C(4)—C(10)—C(9)	116.9 (2)
C(3)—C(4)—C(10)	121.3 (2)	C(4)—C(10)—C(5)	126.7 (2)
C(10)—C(4)—C(16)	120.1 (2)	C(7)—N(12)—C(13)	123.1 (2)
C(6)—C(5)—C(10)	122.7 (2)	N(12)—C(13)—C(14)	111.2 (2)
C(5)—C(6)—C(15)	120.6 (2)	C(4)—C(16)—F(19)	111.3 (2)
C(5)—C(6)—C(7)	119.3 (2)	C(4)—C(16)—F(18)	112.1 (2)
C(7)—C(6)—C(15)	120.1 (2)	C(4)—C(16)—F(17)	112.6 (2)
C(6)—C(7)—N(12)	120.3 (2)	F(18)—C(16)—F(19)	106.5 (2)
C(6)—C(7)—C(8)	118.7 (2)	F(17)—C(16)—F(19)	107.1 (2)
C(8)—C(7)—N(12)	120.9 (2)	F(17)—C(16)—F(18)	106.9 (2)
C(7)—C(8)—C(9)	120.0 (2)		

shown in Fig. 1. The final fractional atomic coordinates and the equivalent isotropic temperature factors for the non-H atoms are given in Table 1; the bond lengths and bond angles involving these atoms are listed in Table 2.*

* List of structure factors, anisotropic thermal parameters, H-atom coordinates, distances and angles involving H atoms, torsion angles, least-squares planes and intermolecular distances less than 3.5 Å have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54491 (19 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: MU0271]

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Structure of 1-(3-Deoxy-3-phenylseleno-2,5-di-O-pivaloyl-β-D-xylofuranosyl)uracil

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Abstract. C₂₅H₂₃N₂O₇Se, *M_r* = 542.43, monoclinic, *C*2, *a* = 21.078 (1), *b* = 7.036 (2), *c* = 19.603 (1) Å, β = 109.05 (1)°, *V* = 2748.1 (7) Å³, *Z* = 4, *D_x* = 1.311 Mg m⁻³, λ(Cu Kα₁) = 1.54050 Å, μ = 2.238 mm⁻¹, *F*(000) = 1108, *T* = 295 K, final *R* = 0.037 for 2191 reflections. The sugar conformation

Related literature. The title compound, a laser dye also known as coumarin 503, has been found to give laser emissions around 503 nm in alcohols (Drexhage & Reynolds, 1974; Reynolds & Drexhage, 1975). The structural study was performed as part of our program on the structural aspects of aminocoumarin laser dyes. The structural details of related aminocoumarin dyes have been published elsewhere (Messenger & Delugeard, 1974; Chinnakali, Sivakumar & Natarajan, 1989, 1990; Chinnakali, Selladurai, Sivakumar, Subramanian & Natarajan, 1990).

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and puckering parameters are ²*E* with *P* = −15.8° and ψ_{*m*} = 40.3°. The N-glycosidic torsion angle χ has a value of 142.6 (4)° in the *anti* range. The C4'—C5' side-chain conformation is *-ap* with γ = −175.7 (6)°. The conformation parameters are in accordance with the IUPAC–IUB Joint Commission

Table 1. Atomic coordinates and equivalent isotropic thermal parameters (Å²)
$$B_{\text{eq}} = (1/3) \sum_i \sum_j B_{ij} a_i^* a_j^* a_i \cdot a_j.$$

	x	y	z	B _{eq}
N1	1.0690 (2)	0.6089 (7)	0.3552 (2)	3.59 (14)
C2	1.1077 (2)	0.7660 (9)	0.3867 (3)	3.61 (16)
O2	1.0908 (1)	0.9251 (9)	0.3693 (2)	5.17 (13)
N3	1.1666 (2)	0.7192 (7)	0.4395 (2)	3.58 (13)
C4	1.1904 (3)	0.5403 (9)	0.4621 (3)	3.78 (17)
O4	1.2454 (2)	0.5248 (6)	0.5104 (2)	4.60 (12)
C5	1.1488 (3)	0.3858 (9)	0.4261 (3)	4.19 (18)
C6	1.0911 (2)	0.4250 (12)	0.3744 (2)	4.16 (16)
C1'	1.0083 (2)	0.6442 (9)	0.2941 (3)	3.50 (15)
C2'	1.0152 (2)	0.6021 (9)	0.2218 (2)	3.62 (15)
O2'	1.0400 (2)	0.7631 (6)	0.1935 (2)	4.19 (12)
C3'	0.9427 (2)	0.5601 (10)	0.1752 (2)	3.71 (16)
Se3'	0.94452 (3)	0.41772*	0.09052 (3)	4.98 (2)
C4'	0.9140 (2)	0.4681 (9)	0.2297 (3)	3.78 (18)
O4'	0.9588 (1)	0.5149 (6)	0.3006 (1)	4.17 (11)
C5'	0.9066 (4)	0.2569 (12)	0.2253 (4)	5.23 (24)
O5'	0.8839 (2)	0.2046 (7)	0.2846 (2)	6.16 (17)
C21'	1.1063 (3)	0.7636 (11)	0.2000 (4)	4.38 (21)
O21'	1.1425 (2)	0.6351 (8)	0.2284 (3)	7.29 (22)
C22'	1.1253 (2)	0.9431 (12)	0.1702 (3)	4.87 (19)
C23'	1.1100 (6)	1.1131 (14)	0.2108 (6)	6.99 (38)
C24'	1.0839 (5)	0.9531 (19)	0.0893 (4)	7.46 (33)
C25'	1.2001 (3)	0.9342 (19)	0.1813 (5)	7.00 (28)
C31'	0.8556 (2)	0.4536 (10)	0.0253 (2)	4.08 (17)
C32'	0.8471 (3)	0.4438 (13)	-0.0470 (3)	5.29 (20)
C33'	0.7826 (4)	0.4493 (13)	-0.0973 (3)	6.19 (24)
C34'	0.7281 (4)	0.4659 (11)	-0.0746 (4)	5.85 (24)
C35'	0.7360 (3)	0.4813 (11)	-0.0032 (4)	5.58 (24)
C36'	0.8002 (3)	0.4730 (10)	0.0479 (3)	4.88 (20)
C51'	0.8712 (2)	0.0207 (10)	0.2903 (3)	4.23 (18)
O51'	0.8738 (2)	-0.0923 (9)	0.2462 (2)	5.75 (14)
C52'	0.8544 (3)	-0.0198 (11)	0.3589 (3)	5.34 (23)
C53'	0.9176 (5)	-0.0703 (55)	0.4157 (6)	15.44 (83)
C54'	0.8196 (9)	0.1478 (24)	0.3799 (9)	13.26 (71)
C55'	0.8063 (11)	-0.1861 (27)	0.3463 (8)	-14.04 (84)

* Origin-defining parameter.

Table 2. Selected bond lengths (Å) and angles (°)

N1—C6	1.384 (9)	N1—C2	1.393 (8)
N1—C1'	1.461 (6)	C2—O2	1.190 (9)
C2—N3	1.372 (6)	N3—C4	1.373 (8)
C4—O4	1.239 (6)	C4—C5	1.430 (8)
C5—C6	1.334 (7)	C6—C5	1.334 (7)
C1'—O4'	1.421 (7)	C1'—C2'	1.501 (9)
C2'—O2'	1.433 (8)	C2'—C3'	1.532 (6)
O2'—C21'	1.363 (9)	C3'—C4'	1.531 (9)
C3'—Se3'	1.950 (6)	Se3'—C31'	1.909 (5)
C4'—O4'	1.442 (6)	C4'—C5'	1.494 (11)
C5'—O5'	1.441 (11)	O5'—C51'	1.334 (9)
C21'—O21'	1.195 (9)	C21'—C22'	1.499 (12)
C51'—O51'	1.188 (9)	C51'—C52'	1.524 (10)
C6—N1—C2	121.7 (4)	C6—N1—C1'	120.5 (4)
C2—N1—C1'	117.3 (4)	O2—C2—N3	123.7 (5)
O2—C2—N1	122.8 (4)	N3—C2—N1	113.5 (5)
C2—N3—C4	127.5 (5)	O4—C4—N3	118.6 (5)
O4—C4—C5	125.5 (6)	N3—C4—C5	115.9 (4)
C6—C5—C4	118.6 (6)	C5—C6—N1	122.8 (6)
O4'—C1'—N1	106.8 (4)	O4'—C1'—C2'	105.0 (4)
N1—C1'—C2'	114.3 (5)	O2'—C2'—C1'	111.7 (5)
O2'—C2'—C3'	109.9 (4)	C1'—C2'—C3'	102.4 (4)
C21'—O2'—C2'	117.3 (5)	C4'—C3'—C2'	102.2 (4)
C4'—C3'—Se3'	119.9 (4)	C2'—C3'—Se3'	108.3 (4)
C31'—Se3'—C3'	102.4 (2)	O4'—C4'—C5'	107.8 (5)
O4'—C4'—C3'	107.0 (4)	C5'—C4'—C3'	116.1 (6)
C1'—O4'—C4'	109.1 (4)	O5'—C5'—C4'	105.4 (6)
C51'—O5'—C5'	116.4 (6)	O21'—C21'—O2'	121.3 (7)
O21'—C21'—C22'	127.4 (7)	O2'—C21'—C22'	111.2 (6)
O51'—C51'—O5'	122.0 (6)	O51'—C51'—C52'	126.5 (7)
O5'—C51'—C52'	111.5 (6)		

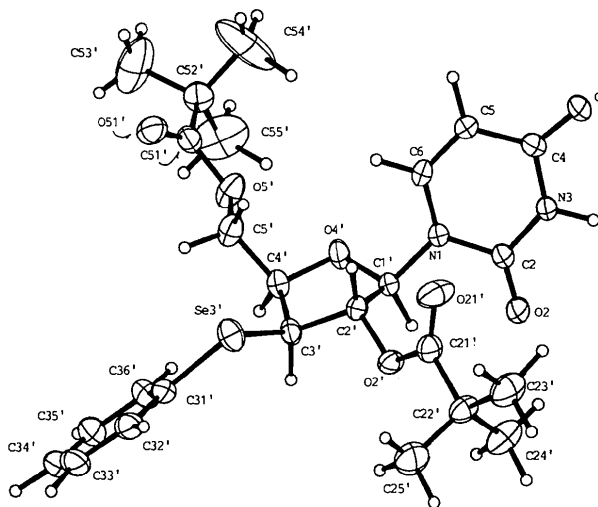


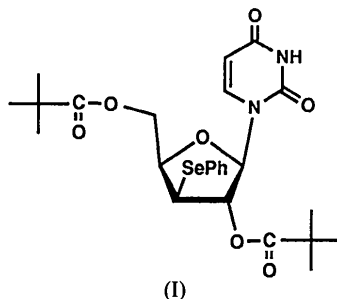
Fig. 1. ORTEP drawing of (I). Ellipsoids are drawn at the 50% probability level while isotropic H thermal parameters are represented by spheres of arbitrary size.

on Biochemical Nomenclature [Pure Appl. Chem. (1983), 55, 1273–1280] guidelines.

Experimental. The title compound (I) has recently been prepared by nucleophilic substitution of the 3'-mesyloxy group with the phenylselenide anion. Crystal dimensions 0.30 × 0.20 × 0.55 mm, by recrystallization from CH₃COOC₂H₅/CH₃(CH₂)₄CH₃ having m.p. 431–433 K. Rigaku AFC-5 four-circle diffractometer used with ω-2θ-scan method, ω-scan width (1.3 + 0.14tanθ)° and scan speed 16° min⁻¹. Lattice parameters obtained from least-squares analysis of 20 reflections with 2θ values ranging from 58 to 61°. Of 2363 reflections scanned [within index range *h* -23–23, *k* 0–7, *l* 0–22 up to sinθ/λ < 0.56 Å⁻¹ including 72 equivalent reflections (*R*_{int} = 0.012)], 2242 unique reflections [*F* > σ(*F*)] classified as observed. Three standard reflections measured every 150 reflections, intensity variation < 3%. Intensities corrected for Lorentz and polarization factors, but absorption correction not applied. Structure solved using program package SAPI85 (Yao, Zheng, Qian, Han, Gu & Fan, 1985). The refinement was carried out by the full-matrix least-squares method with anisotropic temperature factors for non-H atoms. The function minimized was $\sum w[(|F_o|)^2 - (|F_c|)^2]^2$ with $w = 1/[\sigma^2(F_o) +$

0.008(*F_o*), σ(*F_o*) determined from counting statistics. All H atoms located from a difference map and theoretical calculations were refined, initial thermal parameters set at equivalent isotropic thermal parameters of each bonded atom. Final discrepancy indices *R* = 0.037, *wR* = 0.045, *S* = 2.910 for 443 variables and 2191 reflections with *F* > 3σ(*F*). Maximum Δ/σ = 0.40 in final least-squares cycle. Final difference Fourier excursions 0.24 and -0.20 e Å⁻³. All major computations performed on a PANAFACOM computer with the RCRYSTAN (Rigaku

Corporation, 1985) X-ray analysis program system. The atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV).



Final atomic parameters are listed in Table 1.* Selected bond lengths and angles are listed in Table 2. Fig. 1 shows an ORTEP drawing (Johnson, 1976) of the molecule with its atom labels.

Related literature. Nucleosides containing a phenylseleno group in the sugar portion constitute useful

* Tables of H-atom coordinates, anisotropic thermal parameters and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54494 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS0514]

synthons for the preparation of anti-HIV agents (Vial, Agback & Chattopadhyaya, 1990; Chu, Babu, Beach, Ahn, Huang, Jeong & Lee, 1990; Cosford & Schinazi, 1991). Determination of the stereochemistry of the phenylseleno group is an important step, since the subsequent selenoxide fragmentation is known to be stereospecific *syn*-elimination. The title compound has been used for the synthesis of 2'- and 3'-carbon substituted nucleoside derivatives (Haraguchi, Tanaka, Itoh & Miyasaka, 1991).

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Structure of Terphenyldiol Dibenzoate

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Abstract. *m*-Terphenyl-4,4'-diyl dibenzoate, C₃₂H₂₂O₄, *M_r* = 470.5, orthorhombic, *P*2₁2₁2₁, *a* = 6.720 (3), *b* = 11.618 (6), *c* = 30.452 (12) Å, *V* = 2377 Å³, *Z* = 4, *D_x* = 1.314 g cm⁻³, λ(Mo *K*α) = 0.71069 Å, μ = 0.8 cm⁻¹, *F*(000) = 984, *T* = 203 K, *R* = 0.0558 for 4354 unique reflections with *I* > 4σ(*I*). A symmetric molecule with nonplanar phenyl groups. The two outer phenyl groups are rotated out of the central phenyl plane by 26.3° (C1–C6) and 23.4° (C27–C32). The remaining two phenyl groups are rotated out of the central phenyl plane by 33.0° (C8–C13) and 30.9° (C20–C25).

Experimental. Compound obtained by reaction of 4,4'-dihydroxy-1,1':3',1''-terphenyl with benzoyl chloride in the presence of pyridine and recrystallized from a toluene solution at 253 K. Crystal sealed in glass capillary for low-temperature data collection. Siemens *R3m/V* upgrade of Nicolet *P3F* automated diffractometer, 2θ–θ scan with variable scan speeds. Structure solved by direct methods and refined on *F* using *SHELXTL-plus* (Sheldrick, 1988) on a MicroVAX II computer. H atoms were placed in idealized positions, and constrained to have C–H = 0.96 Å and isotropic thermal parameters, *U* = 0.08 Å². All non-H atoms treated as anisotropic. No absorption correction was applied. Details of the data collection

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