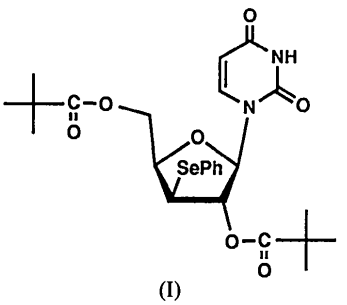
Corporation, 1985) X-ray analysis program system. The atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV).



(I)

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

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

* 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]

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Structure of Terphenyldiol Dibenzoate

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Abstract. *m*-Terphenyl-4,4″-diyl dibenzoate, $C_{32}H_{22}O_4$, $M_r = 470.5$, orthorhombic, $P2_12_12_1$, $a = 6.720\ (3)$, $b = 11.618\ (6)$, $c = 30.452\ (12)$ Å, $V = 2377$ Å^3, $Z = 4$, $D_x = 1.314$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 0.8$ cm^{-1}, $F(000) = 984$, $T = 203$ K, $R = 0.0558$ for 4354 unique reflections with $I > 4\sigma(I)$. 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 *R*3*m*/*V* upgrade of Nicolet *P*3*F* 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, $U = 0.08$ Å^2. All non-H atoms treated as anisotropic. No absorption correction was applied. Details of the data collection

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Table 1. *Experimental details*

Crystal	
Habit	Prism
Size (mm)	0.20 × 0.20 × 0.20
Lattice parameters	
Number of reflections	44
2θ range (°)	6.63–29.32
Reflection range	
h	−8 to 8
k	0 to 15
l	0 to 39
Max. $\sin\theta/\lambda$ (Å^{-1})	0.650
Check reflections, variation (%)	$\bar{1}02,1\bar{1}6,0\bar{1}8$ 5,5,3
Number of reflections	
Collected	5839
Unique observed	4354
R_{int}	0.023
Observed criterion	$I > 4\sigma(I)$
Number of parameters	327
R, wR	0.056, 0.073
S	1.08
Secondary-extinction parameter (χ), $F^* = F[1 + 0.002\chi F^2/\sin(2\theta)]^{-1/4}$	0.006 (3)
Weighting factor (g), $w^{-1} = \sigma^2(F) + gF^2$	0.0027
Fourier difference peaks	
Min., max. (e Å^{-3})	−0.43, 0.52
Max. Δ/σ	0.025

Table 3. *Torsion angles* (°)

C6—C1—C2—C3	−1.7 (4)	C7—C1—C2—C3	177.1 (3)
C2—C1—C6—C5	2.3 (4)	C7—C1—C6—C5	−176.5 (3)
C2—C1—C7—O1	0.8 (4)	C2—C1—C7—O2	−177.8 (2)
C6—C1—C7—O1	179.6 (3)	C6—C1—C7—O2	1.0 (4)
C1—C2—C3—C4	0.0 (5)	C2—C3—C4—C5	1.1 (5)
C3—C4—C5—C6	−0.5 (5)	C4—C5—C6—C1	−1.2 (5)
C1—C7—O2—C8	174.3 (2)	O1—C7—O2—C8	−4.3 (4)
C7—O2—C8—C9	129.1 (3)	C7—O2—C8—C13	−55.3 (3)
O2—C8—C9—C10	175.0 (2)	C13—C8—C9—C10	−0.6 (4)
O2—C8—C13—C12	−175.2 (2)	C9—C8—C13—C12	0.2 (4)
C8—C9—C10—C11	0.9 (4)	C9—C10—C11—C12	−1.0 (4)
C9—C10—C11—C14	−179.6 (3)	C10—C11—C12—C13	0.6 (4)
C14—C11—C12—C13	179.3 (3)	C10—C11—C14—C15	33.2 (4)
C10—C11—C14—C19	−150.0 (3)	C12—C11—C14—C15	−145.4 (3)
C12—C11—C14—C19	31.3 (4)	C11—C12—C13—C8	−0.3 (4)
C11—C14—C15—C16	175.8 (2)	C19—C14—C15—C16	−1.0 (4)
C11—C14—C19—C18	−176.4 (3)	C15—C14—C19—C18	0.4 (4)
C14—C15—C16—C17	1.0 (4)	C14—C15—C16—C20	−176.7 (2)
C15—C16—C17—C18	−0.4 (4)	C20—C16—C17—C18	177.3 (3)
C15—C16—C20—C21	−31.0 (4)	C15—C16—C20—C25	147.4 (3)
C17—C16—C20—C21	151.3 (3)	C17—C16—C20—C25	−30.2 (4)
C16—C17—C18—C19	−0.1 (4)	C17—C18—C19—C14	0.1 (4)
C16—C20—C21—C22	180.0 (2)	C25—C20—C21—C22	1.5 (4)
C16—C20—C25—C24	−179.6 (2)	C21—C20—C25—C24	−1.1 (4)
C20—C21—C22—C23	−1.2 (4)	C21—C22—C23—C24	0.5 (4)
C21—C22—C23—O3	−174.9 (2)	C22—C23—C24—C25	−0.1 (4)
O3—C23—C24—C25	175.1 (2)	C22—C23—O3—C26	−128.8 (3)
C24—C23—O3—C26	55.8 (3)	C23—C24—C25—C20	0.5 (4)
C23—O3—C26—O4	4.0 (4)	C23—O3—C26—C27	−176.3 (2)
O3—C26—C27—C28	−3.2 (4)	O3—C26—C27—C32	175.2 (2)
O4—C26—C27—C28	176.5 (3)	O4—C26—C27—C32	−5.1 (4)
C26—C27—C28—C29	177.4 (3)	C32—C27—C28—C29	−0.9 (4)
C26—C27—C32—C31	177.8 (3)	C28—C27—C32—C31	0.7 (4)
C27—C28—C29—C30	0.2 (4)	C28—C29—C30—C31	0.8 (5)
C29—C30—C31—C32	−1.1 (5)	C30—C31—C32—C27	0.3 (4)

Table 2. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* (Å$^2 \times 10^4$)

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

	x	y	z	U_{eq}
C(1)	8035 (4)	5786 (3)	1209 (1)	264 (8)
C(2)	8851 (5)	4842 (2)	1420 (1)	300 (9)
C(3)	7701 (5)	4204 (3)	1709 (1)	361 (10)
C(4)	5736 (5)	4511 (3)	1787 (1)	358 (10)
C(5)	4909 (5)	5448 (3)	1570 (1)	339 (9)
C(6)	6052 (5)	6083 (3)	1277 (1)	291 (8)
C(7)	9372 (4)	6470 (2)	919 (1)	247 (8)
C(8)	9501 (4)	8183 (2)	497 (1)	232 (7)
C(9)	8777 (4)	8478 (2)	88 (1)	236 (7)
C(10)	9732 (4)	9325 (2)	−153 (1)	231 (8)
C(11)	11428 (4)	9871 (2)	10 (1)	211 (7)
C(12)	12118 (4)	9552 (2)	425 (1)	227 (7)
C(13)	11171 (4)	8711 (3)	670 (1)	253 (8)
C(14)	12488 (4)	10790 (2)	−238 (1)	215 (7)
C(15)	11459 (4)	11553 (2)	−508 (1)	205 (7)
C(16)	12411 (4)	12464 (2)	−720 (1)	212 (7)
C(17)	14463 (4)	12595 (2)	−662 (1)	250 (8)
C(18)	15502 (4)	11837 (3)	−398 (1)	271 (8)
C(19)	14530 (4)	10942 (2)	−187 (1)	241 (8)
C(20)	11284 (4)	13310 (2)	−988 (1)	205 (7)
C(21)	9555 (4)	13004 (2)	−1214 (1)	229 (7)
C(22)	8520 (4)	13810 (2)	−1464 (1)	247 (8)
C(23)	9185 (4)	14924 (2)	−1481 (1)	229 (7)
C(24)	10882 (4)	15269 (2)	−1257 (1)	244 (8)
C(25)	11912 (4)	14454 (2)	−1011 (1)	235 (7)
C(26)	8878 (4)	16403 (2)	−2020 (1)	245 (8)
C(27)	7451 (4)	17248 (2)	−2204 (1)	224 (8)
C(28)	5447 (4)	17276 (3)	−2080 (1)	267 (8)
C(29)	4207 (5)	18118 (3)	−2251 (1)	321 (9)
C(30)	4956 (5)	18918 (3)	−2543 (1)	321 (8)
C(31)	6925 (5)	18888 (3)	−2674 (1)	328 (9)
C(32)	8182 (4)	18051 (3)	−2502 (1)	269 (8)
O(1)	11087 (3)	6259 (2)	851 (1)	360 (7)
O(2)	8406 (3)	7389 (2)	747 (1)	267 (6)
O(3)	8003 (3)	15727 (2)	−1707 (1)	260 (6)
O(4)	10575 (3)	16308 (2)	−2128 (1)	348 (7)

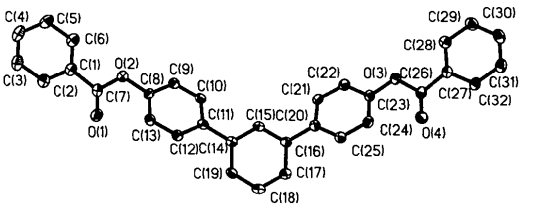

Fig. 1. Thermal-ellipsoid (50% probability) plot.

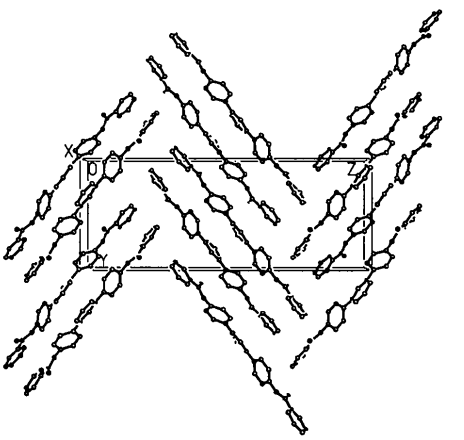

Fig. 2. Projected packing plot viewed down the *a* axis.

are given in Table 1. Scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). Atomic coordinates are contained in Table 2.* Torsion angles for the molecule are contained in Table 3. Fig. 1 illustrates the molecule with the numbering scheme employed. Fig. 2 illustrates the projected packing of the molecules viewed down the *a* axis.

Related literature. For additional information on related compounds, see Karmyshava, Kovshev & Titiov (1976).

* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54445 (25 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF Reference: CR0337]

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Structure of Glycine–Selenious Acid (1/1)

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Abstract. $C_2H_5NO_2.H_2SeO_3$, $M_r = 204.04$, monoclinic, $P2_1/n$, $a = 5.049$ (1), $b = 13.677$ (2), $c = 8.664$ (1) Å, $\beta = 94.92$ (1)°, $V = 596.1$ (1) Å^3, $Z = 4$, $D_m = 2.26$ (1), $D_x = 2.27$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 6.19$ mm^{-1}, $F(000) = 400$, $T = 295$ K, $R = 0.033$ for 870 unique observed reflections. The structure consists of selenious acid dimers and glycine molecules linked together with hydrogen bonds.

Experimental. Molar ratios of 1:2:3.2 with respect to glycine, H_2SeO_3 and H_2O were found from a solubility study to give an optimal yield of the compound $H_3NCH_2COO.H_2SeO_3$. The compound was filtered under suction on a frit, washed with water and dried in air. Colourless crystals were obtained which were stable in air and X-rays. The density was determined pycnometrically.

Data collection and structure refinement parameters are listed in Table 1. The structure was solved by Patterson and Fourier techniques and anisotropically refined by block-diagonal least squares in two blocks. Hydrogen atoms were localized from a $\Delta\rho$ map. All hydrogen atoms were isotropically refined. An empirical absorption correction was applied (Walker & Stuart, 1983), absorption factors varied from 0.797 to 1.603. Atomic parameters are given in Table 2,* details of the molecular geometry and hydrogen bonds are given in Table 3. Figs. 1 and 2 show the molecules of glycine and the selenious acid dimer respectively; the crystal packing is shown in Fig. 3.

Related literature. The study of the title compound was undertaken as part of a systematic investigation of the glycine–selenious acid–water system. This

* Lists of structure factors, anisotropic thermal parameters, H-atom postions and isotropic thermal parameters and bond distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54463 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI0090]

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