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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Table 1. *Data collection and structure refinement parameters*

Crystal dimensions (mm)	0.55 × 0.40 × 0.23
Diffractometer and radiation used (Å)	Enraf–Nonius CAD-4, graphite monochromator λ(Mo Kα) = 0.71073
Scan technique	ω/2θ
Number and θ range (°) of reflections for the refinement of lattice parameters	20; 22.78–24.52
Range of h, k and l	−6→6, −16→16, −10→10
Maximum value of $(\sin\theta)/\lambda$ (Å^{-1})	0.595
Standard reflections	$\bar{1}0\bar{1}$, $\bar{2}11$
Standard reflections with monitoring interval (min), intensity fluctuation (%)	60, −0.5
Total number of reflections measured	3478
2θ range (°)	$2\theta < 50$
R_{int}	0.031
Number of unique observed reflections	870
Criterion for observed reflections	$I > 1.96\sigma(I)$
Function minimized	$\sum w(\|F_o\| - \|F_c\|)^2$
Weighting scheme	$w = 1/[\sigma^2(F_o) + 0.0009F^2]$
Parameters refined	110
R	0.033
wR	0.033
S	1.03
Ratio of maximum least-squares shift to e.s.d. in the last cycle	0.001
Maximum and minimum heights in final $\Delta\rho$ map (e Å^{-3})	0.40, −1.16
Source of atomic scattering factors	*SHELX*76
Programs used	*SDP* (Frenz, 1985), *SHELX*76 (Sheldrick, 1976), *PARST* (Nardelli, 1988)
Computers used	PDP11/73, PC AT 286

Table 2. *Atomic coordinates* (× 10^4) *for non-hydrogen atoms and equivalent isotropic thermal parameters* (× 10^4)

$$U_{eq} = (1/3)[U_{22} + 1/\sin^2\beta(U_{11} + U_{33} + 2U_{13}\cos\beta)].$$

	x	y	z	U_{eq} (Å^2)
Se	2049.3 (7)	43.8 (3)	−2101.5 (4)	215 (1)
O1	1137 (5)	3401 (2)	−1034 (3)	240 (7)
O2	−2567 (5)	3631 (2)	159 (3)	266 (8)
O11	1245 (5)	1004 (2)	−1089 (3)	255 (7)
O22	2582 (6)	−856 (2)	−703 (4)	309 (8)
O33	−1139 (6)	−256 (3)	−2808 (4)	365 (9)
N	3542 (7)	2353 (3)	1255 (4)	209 (9)
C1	−177 (7)	3342 (3)	101 (4)	192 (9)
C2	1123 (8)	2888 (3)	1575 (4)	201 (10)

Table 3. *Bond lengths* (Å), *angles* (°) *and intermolecular hydrogen bonds* (Å, °)

Se—O11	1.649 (3)	O22—Se—O33	99.4 (2)
Se—O22	1.732 (3)	O11—Se—O33	96.5 (1)
Se—O33	1.722 (3)	O11—Se—O22	103.0 (2)
O1—C1	1.235 (5)	O1—C1—O2	125.9 (3)
O2—C1	1.275 (4)	O2—C1—C2	115.9 (3)
N—C2	1.470 (6)	O1—C1—C2	118.3 (3)
C1—C2	1.518 (5)	N—C2—C1	110.6 (3)

O22···O11^{i}	2.588 (4)	O22—HO22···O11^{i}	177 (5)
O33···O2^{ii}	2.582 (4)	O33—HO33···O2^{ii}	166 (5)
N···O2^{iii}	2.852 (5)	N—H1N···O2^{iii}	178 (4)
N···O11^{iv}	2.910 (5)	N—H2N···O11^{iv}	164 (4)
N···O1^{v}	2.787 (4)	N—H3N···O1^{v}	167 (5)

Symmetry code: (i) $-x, -y, -z$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x-1, y, z$; (iv) $x, y+1, z$; (v) $x-\frac{1}{2}, -y+\frac{1}{2}+1, z-\frac{1}{2}$.

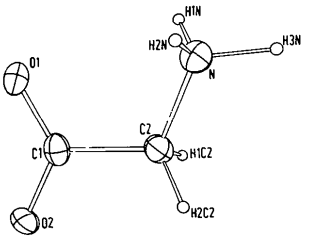

Fig. 1. View of the molecule of glycine with atom numbering. Thermal ellipsoids are scaled to 50% probability.

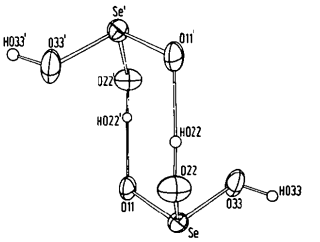

Fig. 2. View of the dimer of selenious acid with atom numbering. Thermal ellipsoids are scaled to 50% probability. Symmetry code: (i) $-x, -y, -z$.

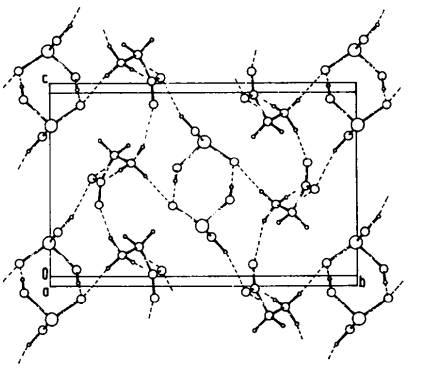

Fig. 3. Packing scheme. Hydrogen bonds are designated by dashed lines.

system is interesting from the point of view of the possibility of forming compounds with ferroelectric properties. The structures of the related compounds triglycine sulfate (Kay & Kleinberg, 1973) and diglycine selenate (Olejnik & Luhaszewisz, 1975) have been determined.

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