N atom. There are no interactions between the molecules exceeding van der Waals forces.

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Structure of (2*S*,3*R*)-3-Amino-2-phenylthiobutanoic Acid

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Abstract. $C_{10}H_{13}NO_2S$, $M_r = 211{\cdot}28$, orthorhombic, $P2_12_12_1$, $a = 8{\cdot}723\ (2)$, $b = 19{\cdot}337\ (4)$, $c = 6{\cdot}365\ (2)$ Å, $V = 1073{\cdot}6\ (5)$ Å^3, $Z = 4$, $D_x = 1{\cdot}307$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ(Mo $K\alpha$) = 0·27 mm^{-1}, $F(000) = 448$, $T = 295$ K, $R = 0{\cdot}032$ for 1147 observed reflections [$F_o > 3\sigma(F_o)$]. The absolute configuration of C(2) was determined as *S* based on the *R* configuration of C(3) which was already known. The molecule adopts the zwitterion form with $-COO^-$ and $-NH_3^+$ groups. The H atoms in $-NH_3^+$ form hydrogen bonds with the O atoms in the $-COO^-$ group; (N4)H''···O(7) (x, y, z) = 1·90 (3) [N···O 2·700 (3)], (N4)H···O(7) ($x-\frac{1}{2}$, $\frac{3}{2}-y$, $1-z$) = 1·94 (3) [2·818 (3)] and (N4)H'···O(8) (x, y, $1+z$) = 1·97 (3) Å [2·788 (3) Å].

Experimental. Prismatic colorless crystals obtained from methanol–water. Crystal of dimensions 0·2 × 0·2 × 0·5 mm. Rigaku AFC-5R diffractometer, graphite-monochromatized Mo $K\alpha$ radiation. Cell dimensions determined from 2θ angles in the range $15 < 2\theta < 24°$. Intensities measured up to $2\theta = 52°$ in h 0/10, k 0/23 and l 0/7, ω–2θ scans, ω-scan width $(1{\cdot}0 + 0{\cdot}45\tan\theta)°$, three standard reflections monitored every 100 measurements showed no significant change. 1214 unique reflections measured, 1147 intensities observed [$F_o \leq 3\sigma(F_o)$ and four very strong reflections rejected], no absorption corrections. Structures solved by *MULTAN*84 (Main, Germain & Woolfson, 1984). H atoms located on a difference density map. Positional parameters of all atoms and anisotropic thermal parameters of non-H atoms refined by block-diagonal

Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å^2) *with e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
S(1)	0·5214 (1)	0·60192 (3)	0·1716 (1)	3·56 (1)
C(2)	0·5626 (2)	0·6748 (1)	0·3441 (3)	2·62 (4)
C(3)	0·5744 (2)	0·6517 (1)	0·5753 (3)	2·91 (4)
N(4)	0·5791 (2)	0·7155 (1)	0·7083 (2)	3·16 (4)
C(5)	0·7121 (3)	0·6059 (1)	0·6227 (3)	4·27 (6)
C(6)	0·7075 (2)	0·7132 (1)	0·2655 (3)	2·76 (4)
O(7)	0·7745 (2)	0·7503 (1)	0·3967 (2)	4·66 (4)
O(8)	0·7469 (2)	0·7067 (1)	0·0802 (2)	3·48 (3)
C(9)	0·3183 (2)	0·5951 (1)	0·1901 (3)	2·91 (4)
C(10)	0·2474 (3)	0·5569 (1)	0·3421 (4)	4·36 (6)
C(11)	0·0889 (3)	0·5503 (1)	0·3433 (5)	5·31 (7)
C(12)	0·0025 (3)	0·5812 (1)	0·1912 (5)	4·66 (6)
C(13)	0·0720 (3)	0·6196 (1)	0·0377 (5)	4·67 (6)
C(14)	0·2301 (3)	0·6268 (1)	0·0357 (4)	4·03 (5)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

S(1)–C(2)	1·822 (2)	C(6)–O(8)	1·235 (3)
S(1)–C(9)	1·780 (2)	C(9)–C(10)	1·365 (3)
C(2)–C(3)	1·541 (3)	C(9)–C(14)	1·390 (3)
C(2)–C(6)	1·549 (3)	C(10)–C(11)	1·388 (4)
C(3)–N(4)	1·497 (3)	C(11)–C(12)	1·365 (5)
C(3)–C(5)	1·523 (3)	C(12)–C(13)	1·369 (5)
C(6)–O(7)	1·246 (3)	C(13)–C(14)	1·386 (4)

C(2)–S(1)–C(9)	102·3 (1)	O(7)–C(6)–O(8)	124·6 (2)
S(1)–C(2)–C(3)	111·4 (1)	S(1)–C(9)–C(10)	122·5 (2)
S(1)–C(2)–C(6)	109·7 (1)	S(1)–C(9)–C(14)	118·1 (2)
C(3)–C(2)–C(6)	113·1 (2)	C(10)–C(9)–C(14)	119·3 (2)
C(2)–C(3)–N(4)	107·6 (2)	C(9)–C(10)–C(11)	120·3 (2)
C(2)–C(3)–C(5)	114·2 (2)	C(10)–C(11)–C(12)	120·4 (3)
N(4)–C(3)–C(5)	110·2 (2)	C(11)–C(12)–C(13)	120·0 (3)
C(2)–C(6)–O(7)	116·2 (2)	C(12)–C(13)–C(14)	120·1 (3)
C(2)–C(6)–O(8)	119·1 (2)	C(9)–C(14)–C(13)	120·0 (2)

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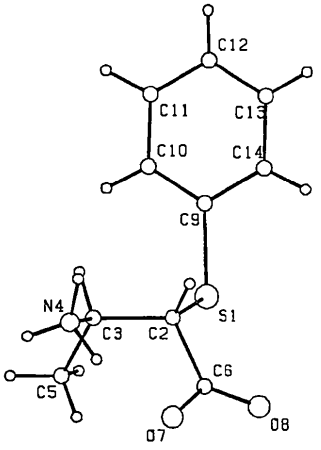

Fig. 1. Perspective view with the atom-numbering system.

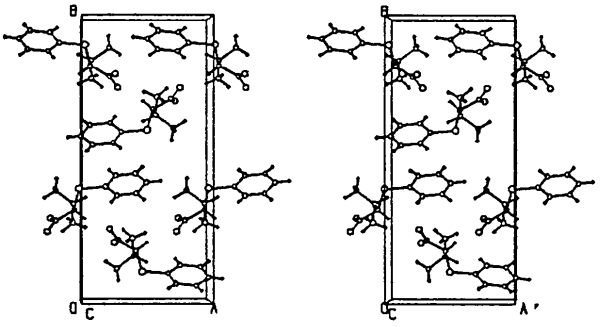

Fig. 2. A stereoview of the unit-cell packing.

least squares. Temperature factor of each H atom equal to B_{eq} of the bonded atom. $\sum(w|\Delta F|^2)$ minimized, $w = 1/[\sigma^2(F_o) + 0{\cdot}00128|F_o|^2]$, $w = 0$ for nine reflections with $w^{1/2}|\Delta F| \geq 3$. Final $R = 0{\cdot}032$, $wR = 0{\cdot}042$, $S = 1{\cdot}0853$. Highest peak in final difference map using the F data of $\theta \leq 18°$ is 0·3 e Å^{-3}. Max. Δ/σ in the final cycle 0·1. Atomic scattering factors calculated by $\sum[a_i\exp(-b_i\lambda^{-2}\sin^2\theta)] + c$ $(i = 1,\ldots,4)$ (*International Tables for X-ray Crystallography*, 1974). Calculations performed on FACOM M340R computer at Shionogi Research Laboratories. The final atomic coordinates and equivalent isotropic temperature factors are given in Table 1. Bond distances and angles are listed in Table 2.* A perspective view of the molecule with the atom-numbering system and a stereoview of the crystal packing drawn using the program *PLUTO* (Motherwell & Clegg, 1978) are presented in Figs. 1 and 2, respectively.

Related literature. The absolute configuration of the title compound reported here has been discussed in Hata & Watanabe (1987).

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* Lists of structure factors, anisotropic temperature factors of the non-H atoms and atomic coordinates of the H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51036 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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rel-(2*S*,6*S*)-2-(6-Hydroxy-4,4,6-trimethyl)morpholinomethanesulfonate

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Abstract. $C_8H_{17}NO_5S$, $M_r = 239{\cdot}3$, orthorhombic, *Pbca*, $a = 11{\cdot}789$ (4), $b = 14{\cdot}679$ (2), $c = 12{\cdot}733$ (1) Å, $V = 2203{\cdot}5$ (8) Å^3, $Z = 8$, $D_x = 1{\cdot}443$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 2{\cdot}8$ cm^{-1}, $F(000) = 1024$, $T = 295$ (1) K, 3005 unique reflections measured, final $R = 0{\cdot}058$ for 1360 reflections having $F_o > 5\sigma(F_o)$. Pairs of zwitterion molecules are bound centrosymmetrically by hydrogen bonds between the hydroxyl group and a sulfonate oxygen (O3): O2···O3 = 2·789 (4), O2–H = 1·05 (1), H···O3 = 1·80 (1) Å,

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