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2-Hydroxy-3-phenyl-3-pyrrolidinylpropionamide

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(*Received* 16 *December* 1977; *accepted* 14 *January* 1978)

Abstract. $C_{13}H_{18}N_2O_2$, monoclinic, $P2_1/c$, a = 7·844 (3), b = 16·619 (7), c = 20·802 (12) Å, β = 103·2 (3)°, V = 2640 (2) Å^3, Z = 8, D_x = 1·179 g cm^{-3}. The compound is an *erythro* phenylisoserine derivative. One molecule of the asymmetric unit forms an N···O hydrogen-bonded dimer with its inversion image; the second is connected to two different dimers by O···O hydrogen bonds. The result is a network of molecules within a layer parallel to (100) of thickness d_{100} = 7·636 Å. The layers are held together by packing forces only.

Introduction. The title compound (Fig. 1) was synthesized by Dr W. Tack and Professor Zymalkowski (Pharmazeutisches Institut der Universität Bonn). A crystal, 0·2 × 0·1 × 0·1 mm, was selected for the diffraction experiments. Intensity measurements were carried out in the ω mode on an automatic Syntex $P2_1$ four-circle diffractometer with Mo $K\alpha$ radiation (λ = 0·71069 Å) monochromatized by a graphite crystal. 3406 reflexions were recorded, resulting in a set of 2921 unique reflexions, of which 887 were regarded as unobserved ($I < 3\sigma$).

No absorption correction was applied (μ = 0·90 cm^{-1}). The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971), which fixed the positions of 33 non-hydrogen atoms in the asymmetric unit. The completion of the structure solution was achieved by Fourier methods and calculation of H

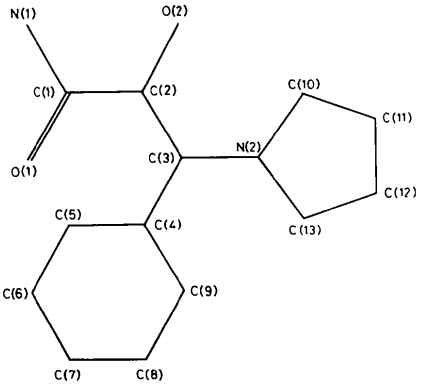

Fig. 1. The numbering scheme.

atom positions. Refinement was by full-matrix least squares with weights $w = 1/\sigma^2(F)$ and anisotropic temperature factors. The H atoms were allocated the isotropic temperature factors of their carrier atoms, but their positions were refined. Owing to the large number of parameters (416) refinement had to take place in overlapping cycles. An isotropic extinction factor g {Zachariasen, 1963; $F_c = kF_o[1 + \beta(2\theta)gI_c]$} was included in the list of variables (final value 7 × 10^{-7}). With six reflexions excluded from refinement the final R

was 0·065 (0·040 omitting unobserveds) and R_w = 0·040 (0·035). The goodness of fit was 1·63.*

Discussion. The reaction of *trans*-3-phenylglycide acid derivatives with primary and secondary amines can lead to either 3-phenylserine or 3-phenylisoserine type compounds (Tack, 1977). Several aminolysis products have been investigated by chemical methods and ^{1}H NMR spectroscopy. However, neither the chemical reactions nor the spectra allowed unambiguous assignment of the reaction products to the phenylserine or phenylisoserine series. In order to classify the products, the molecular configuration of a representative had to be investigated by X-ray diffraction. The title compound (Fig. 1) was chosen because it gave good crystals.

Tables 1 and 2 give the fractional coordinates, and bond distances and angles of molecules (I) and (I′) of the asymmetric unit. An *ORTEP* drawing (Johnson, 1965) of the asymmetric unit is depicted in Fig. 2. The molecule is clearly a phenylisoserine derivative in the *erythro* form. Bond angles and distances are normal. C—H distances vary from 0·91 to 1·01 Å with a mean of 1·01 (4) Å.

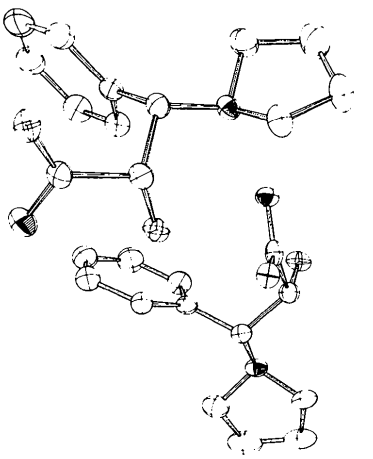

Fig. 2. A perspective view of the asymmetric unit.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33317 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Positional parameters* (*non-hydrogen atoms* × 10^4, H *atoms* × 10^3) *with e.s.d.'s in parentheses*

	x	y	z		x	y	z
C(1)	−103 (5)	3198 (2)	2498 (2)	H(C2)	124 (3)	377 (1)	192 (1)
C(2)	451 (4)	3286 (2)	1846 (1)	H(C3)	261 (3)	255 (1)	217 (1)
C(3)	1576 (3)	2548 (2)	1753 (1)	H(C5)	−84 (4)	184 (2)	81 (1)
C(4)	600 (4)	1761 (2)	1749 (1)	H(C6)	−236 (4)	64 (2)	76 (1)
C(5)	−653 (5)	1517 (2)	1196 (2)	H(C7)	−169 (4)	−24 (2)	173 (1)
C(6)	−1486 (5)	781 (3)	1193 (2)	H(C8)	41 (4)	23 (2)	270 (1)
C(7)	−1091 (5)	291 (2)	1729 (3)	H(C9)	189 (3)	145 (1)	267 (1)
C(8)	120 (5)	530 (2)	2279 (2)	H1(C10)	270 (4)	141 (2)	94 (1)
C(9)	955 (4)	1271 (2)	2291 (2)	H2(C10)	420 (4)	186 (2)	144 (1)
C(10)	3341 (5)	1963 (2)	1047 (2)	H1(C11)	353 (4)	212 (2)	8 (2)
C(11)	4264 (6)	2293 (4)	531 (2)	H2(C11)	525 (4)	200 (2)	56 (2)
C(12)		3189 (3)	608 (2)	H1(C12)	364 (4)	340 (2)	20 (1)
C(13)	3329 (4)	3352 (2)	1156 (2)	H2(C12)	555 (4)	339 (2)	74 (1)
O(1)	1015 (3)	3184 (1)	3021 (1)	H1(C13)	256 (4)	390 (2)	107 (1)
O(2)	−1054 (3)	3380 (1)	1333 (1)	H2(C13)	418 (4)	339 (2)	159 (1)
N(1)	−1805 (3)	3132 (1)	2460 (1)	H(O2)	−80 (3)	349 (2)	97 (1)
N(2)	2220 (3)	2639 (2)	1151 (1)	H1(N1)	−218 (3)	304 (2)	285 (1)
C(1′)	−128 (4)	1142 (2)	4643 (2)	H2(N1)	−259 (3)	312 (2)	203 (1)
C(2′)	−383 (4)	1958 (2)	4318 (1)	H(C2′)	22 (3)	231 (1)	466 (1)
C(3′)	−2381 (4)	2137 (2)	4141 (1)	H(C3′)	−268 (3)	222 (1)	461 (1)
C(4′)	−3417 (4)	1457 (2)	3758 (2)	H(C5′)	−259 (3)	167 (2)	288 (1)
C(5′)	−3381 (4)	1294 (2)	3103 (2)	H(C6′)	−424 (4)	56 (2)	229 (1)
C(6′)	−4324 (5)	658 (2)	2779 (2)	H(C7′)	−597 (4)	−30 (2)	287 (1)
C(7′)	−5316 (5)	175 (2)	3083 (2)	H(C8′)	−603 (4)	−6 (2)	398 (1)
C(8′)	−5372 (5)	325 (2)	3729 (2)	H(C9′)	−437 (3)	109 (2)	453 (1)
C(9′)	−4426 (4)	966 (2)	4065 (2)	H1(C10′)	−190 (4)	353 (2)	464 (1)
C(10′)	−1803 (5)	3593 (2)	4155 (2)	H2(C10′)	−56 (4)	357 (2)	414 (1)
C(11′)	−2865 (6)	4324 (2)	3859 (2)	H1(C11′)	−259 (4)	477 (1)	417 (2)
C(12′)	−4692 (5)	4007 (3)	3592 (2)	H2(C11′)	−239 (4)	452 (2)	345 (2)
C(13′)	−4617 (4)	3118 (2)	3674 (2)	H1(C12′)	−540 (4)	429 (2)	388 (2)
O(1′)	−618 (3)	1019 (1)	5165 (1)	H2(C12′)	−495 (4)	405 (2)	310 (2)
O(2′)	369 (2)	1937 (1)	3760 (1)	H1(C13′)	−504 (4)	301 (2)	412 (1)
N(1′)	637 (3)	582 (1)	4354 (1)	H2(C13′)	−522 (4)	284 (2)	331 (1)
N(2′)	−2730 (3)	2909 (1)	3790 (1)	H(O2′)	58 (3)	252 (2)	360 (1)
				H1(N1′)	74 (3)	0 (2)	453 (1)
				H2(N1′)	95 (3)	78 (2)	397 (1)

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

C(1)–O(1)	1·232 (3)	C(1′)–O(1′)	1·248 (3)	C(1)–C(2)–O(2)	109·0 (2)	C(1′)–C(2′)–O(2′)	107·9 (2)
C(1)–N(1)	1·324 (4)	C(1′)–N(1′)	1·324 (4)	C(3)–C(2)–C(1)	108·8 (2)	C(3′)–C(2′)–C(1′)	107·5 (2)
C(2)–C(1)	1·522 (3)	C(2′)–C(1′)	1·508 (4)	C(3)–C(2)–O(2)	113·2 (2)	C(3′)–C(2′)–O(2′)	113·3 (2)
C(2)–O(2)	1·408 (3)	C(2′)–O(2′)	1·418 (3)	C(2)–C(3)–N(2)	110·1 (2)	C(2′)–C(3′)–N(2′)	110·3 (2)
C(3)–C(2)	1·549 (4)	C(3′)–C(2′)	1·555 (4)	C(4)–C(3)–C(2)	112·5 (2)	C(4′)–C(3′)–C(2′)	112·0 (2)
C(3)–N(2)	1·459 (3)	C(3′)–N(2′)	1·471 (3)	C(4)–C(3)–N(2)	111·0 (2)	C(4′)–C(3′)–N(2′)	112·0 (2)
C(4)–C(3)	1·515 (4)	C(4′)–C(3′)	1·508 (4)	C(5)–C(4)–C(3)	121·2 (3)	C(5′)–C(4′)–C(3′)	122·2 (2)
C(4)–C(5)	1·391 (4)	C(4′)–C(5′)	1·396 (3)	C(5)–C(4)–C(9)	118·7 (3)	C(5′)–C(4′)–C(9′)	118·3 (3)
C(4)–C(9)	1·368 (4)	C(4′)–C(9′)	1·390 (4)	C(9)–C(4)–C(3)	120·2 (2)	C(9′)–C(4′)–C(3′)	119·5 (2)
C(5)–C(6)	1·385 (6)	C(5′)–C(6′)	1·376 (5)	C(4)–C(5)–C(6)	120·3 (3)	C(4′)–C(5′)–C(6′)	120·0 (3)
C(6)–C(7)	1·358 (6)	C(6′)–C(7′)	1·369 (5)	C(5)–C(6)–C(7)	120·4 (3)	C(5′)–C(6′)–C(7′)	121·5 (3)
C(7)–C(8)	1·369 (5)	C(7′)–C(8′)	1·376 (6)	C(6)–C(7)–C(8)	119·8 (4)	C(6′)–C(7′)–C(8′)	119·5 (3)
C(8)–C(9)	1·392 (5)	C(8′)–C(9′)	1·392 (5)	C(7)–C(8)–C(9)	120·3 (3)	C(7′)–C(8′)–C(9′)	119·8 (3)
C(10)–N(2)	1·473 (4)	C(10′)–N(2′)	1·466 (4)	C(8)–C(9)–C(4)	120·4 (1)	C(8′)–C(9′)–C(4′)	120·9 (3)
C(11)–C(10)	1·527 (5)	C(11′)–C(10′)	1·521 (5)	C(11)–C(10)–N(2)	103·0 (3)	C(11′)–C(10′)–N(2′)	104·3 (3)
C(12)–C(11)	1·496 (8)	C(12′)–C(11′)	1·508 (6)	C(12)–C(11)–C(10)	106·0 (3)	C(12′)–C(11′)–C(10′)	104·9 (3)
C(13)–C(12)	1·521 (4)	C(13′)–C(12′)	1·487 (5)	C(13)–C(12)–C(11)	105·4 (3)	C(13′)–C(12′)–C(11′)	107·2 (3)
C(13)–N(2)	1·469 (4)	C(13′)–N(2′)	1·486 (4)	N(2)–C(13)–C(12)	103·9 (3)	N(2′)–C(13′)–C(12′)	105·2 (3)
C(2)–C(1)–O(1)	119·8 (3)	C(2′)–C(1′)–O(1′)	120·2 (2)	C(3)–N(2)–C(10)	112·5 (2)	C(3′)–N(2′)–C(10′)	113·9 (2)
C(2)–C(1)–N(1)	116·3 (2)	C(2′)–C(1′)–N(1′)	117·1 (2)	C(3)–N(2)–C(13)	113·5 (2)	C(3′)–N(2′)–C(13′)	110·5 (2)
O(1)–C(1)–N(1)	123·8 (2)	O(1′)–C(1′)–N(1′)	122·7 (3)	C(13)–N(2)–C(10)	104·1 (2)	C(13′)–N(2′)–C(10′)	105·1 (2)

N–H···O hydrogen bonds are found between (I′) and its inversion image (I′^{i}) with N(1′)–H1(N1′) 1·03 (3), H1(N1′)···O(1′^{i}) 1·82 (3) and N(1′)···O(1′^{i}) 2·844 (3) Å. The angle at H1(N1′) is 173°. Thus (I′) forms dimers around the crystallographic inversion centres at $(0,\frac{1}{2},0)$ and $(0,0,\frac{1}{2})$.

N(1) is not involved in hydrogen bonds, but (I) is connected to a (I′) within the asymmetric unit as well as a (I′) of an adjacent asymmetric unit by O···O hydrogen bonds. These are: O(2)–H(O2)···O(1′^{ii}) with O(2)–H(O2) 0·84 (2), H(O2)···O(1′^{ii}) 1·90 (2) and O(2)···O(1′^{ii}) 2·719 (2) Å; and O(1)···H(O2′)–O(2′) with O(1)···H(O2′) 1·72 (2), H(O2′)–O(2′) 1·05 (3) and O(1)···O(2′) 2·696 Å. The angles around H(O2) and H(O2′) are 165 and 152° respectively. The involvement of O(1′) in two almost perpendicular hydrogen bonds is reflected in the significantly elongated C(1′)=O(1′) distance of 1·248 (3) Å compared with a C(1)=O(1) of 1·232 (3) Å, which corresponds to the expected value.

This arrangement of molecules leads to a layer containing a network of dimers connected *via* molecule (I). Fig. 3 shows a stereoscopic drawing of such a layer viewed approximately along **a**. The layer thickness is d_{100} = 7·636 Å and the layers are held together solely by packing forces.

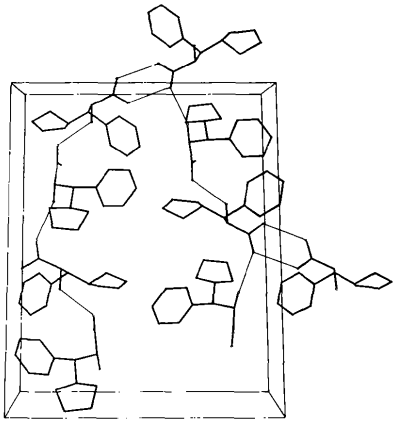

Fig. 3. A perspective view along **a** of a layer of molecules.

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