electron distributions in the amide groups and their different deviations from planarity.

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Structure of (*Z*)-*N*-Acetyl-α,β-didehydrophenylalanyl-L-alanine Hydrate, $C_{14}H_{16}N_2O_4.\frac{1}{3}H_2O$

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Abstract. $M_r = 282\cdot25$, hexagonal, $P6_5$, $a = b = 10\cdot534\ (4)$, $c = 23\cdot753\ (11)$ Å, $V = 2283\ (2)$ Å^3, $Z = 6$, $D_m = 1\cdot230$ (by flotation in aqueous KBr solution), $D_x = 1\cdot232$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0\cdot71069$ Å, $\mu = 0\cdot836$ cm^{-1}, $F(000) = 896$, $T = 298$ K, $R = 0\cdot052$ for 950 reflections with $I > 2\cdot5\sigma(I)$. Molecules, linked by intermolecular hydrogen bonds, are arranged in helices along the *z* axis. The tendency of the phenyl ring to be planar with the C—C—N system causes a change to the expected bond angles. The conformational flexibilities of the saturated and unsaturated amino acids are discussed.

Introduction. Many biologically important peptides contain α,β-unsaturated amino-acid residues which are particularly interesting because of their unusual conformational and electronic features.

In previous papers we reported on the molecular structure of *N*-acetyldehydroalanine (dehydro-Ala-OH) which assumes an extended conformation in the crystal state (Ajò, Granozzi, Tondello, Del Pra & Zanotti, 1979) and, at least as far as the torsion angle φ is concerned, also in the gas phase (Ajò, Granozzi, Ciliberto & Fragalà, 1980). In contrast, we have shown that (*Z*)-*N*-acetyldehydrophenylalanine (dehydro-Phe-OH) is non-planar both in the solid state and in the vapour phase (Ajò, Casarin, Granozzi & Busetti, 1981).

This behaviour is in agreement with theoretical conformational predictions for these compounds having a free or esterified carboxyl group (Ajò, Granozzi, Tondello, Del Pra & Zanotti, 1979; Ajò, Casarin, Granozzi & Busetti, 1981).

The dependence of crystal-state conformation on intermolecular (in particular, hydrogen-bonding) interactions has also been discussed for this class of compounds (Ajò, Busetti, Granozzi & Liakopoulou-Kyriakides, 1984; Ajò, Busetti, Ottenheijm & Plate, 1984).

Conformational studies of dehydrophenylalanine and its derivatives are of interest not only from a biological point of view (Rich & Bhatnagar, 1978, and references therein; Ajò, Granozzi, Tondello & Del Pra, 1980, and references therein) but also in order to investigate the

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mechanism of their asymmetric hydrogenation, which is related to the conformational behaviour of the substrate (Achiwa, Chaloner & Parker, 1981, and references therein; Chan, Pluth & Halpern, 1979; Bacciola, Balestreri, Felicioli, Fissi & Pieroni, 1976; Nakayama, Maeda, Kaneko & Katsura, 1971; Rich & Jasensky, 1979; Sinou, Lafont, Descotes & Kent, 1981).

If the α,β-unsaturated residue is not the carboxy-terminal one the conformational behaviour is quite different: theoretical conformational analysis, carried out by optimizing the conformation of the side chain for each point of the (φ,ψ) map, predicted for the (*Z*)-dehydrophenylalanyl residue (dehydro-Ala-NH-*R*) the existence of six conformational energy minima, none of which corresponds to a planar conformation (Ajò, Casarin & Granozzi, 1982; Ajò, Granozzi, Tondello & Del Pra, 1980).

A systematic investigation is in progress in our laboratory on a series of dehydrophenylalanyl peptides (dehydro-Phe-*X*-OH) with various *X* residues (Ajò, Busetti & Granozzi, 1982).

In the present paper we report on the crystal structure and conformation of (*Z*)-*N*-acetyldehydrophenylalanyl-L-alanine (dehydro-Phe-Ala-OH).*

Experimental. Preparation reported previously (Pieroni, Montagnoli, Fissi, Merlino & Ciardelli, 1975). Needle-shaped crystal 0·15 × 0·15 × 1·00 mm, Philips 1100 four-circle diffractometer, Mo *K*α radiation monochromated by graphite plate, θ–2θ scan mode, scan width 1·2°, scan speed 0·03° s^{-1}, background measured for 7 s at each extremity, θ 2 to 28° ($h \leq 10$, $k \leq 10$, $l \leq 28$); 2 standard intensity and orientation reflections ($1\bar{2}2$) and ($1\bar{1}4$) measured at 3 h intervals: no significant variation; unit cell: least-squares refinement of θ values of 28 high-angles reflections, $20 < \theta < 25°$; 1584 measured reflections, 950 observed [$I > 2{\cdot}5\sigma(I)$]; Lorentz–polarization, no absorption correction; $R_{\rm int} = 2{\cdot}25$. Structure solved by direct methods; full-matrix least-squares refinement (on *F*), anisotropic temperature factors for non-hydrogen atoms, unit weights, $(\Delta/\sigma)_{\rm mean} = 0{\cdot}03$, $(\Delta/\sigma)_{\rm max} = 0{\cdot}09$, $S = 1{\cdot}1$. H atoms located on difference map and included in refinement with isotropic temperature factor, $B = 4{\cdot}0$ Å^2; C(1) methyl-group hydrogen atoms, clearly disordered in two possible positions with occupancy 0·5, were given calculated coordinates. Two water molecules are also present in the unit cell, shared between the six equivalent positions. Residual peaks in final difference map between 0·18 and −0·17 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Programs *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), *SHELX* (Sheldrick, 1976) and *ORTEP*II (Johnson, 1976).

Discussion. An *ORTEP*II drawing of the title compound (dehydro-Phe-Ala-OH) with numbering of atoms and nomenclature of relevant torsion angles is reported in Fig. 1, and final positional parameters are in Table 1.*

Bond distances and angles are shown in Table 2, and the crystal packing is given in Fig. 2.

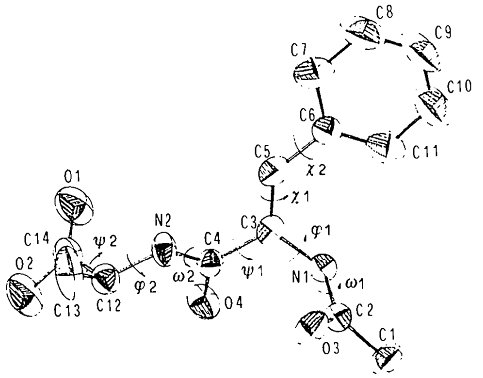

Fig. 1. *ORTEP*II projection of dehydro-Phe-Ala-OH viewed along the *z* axis.

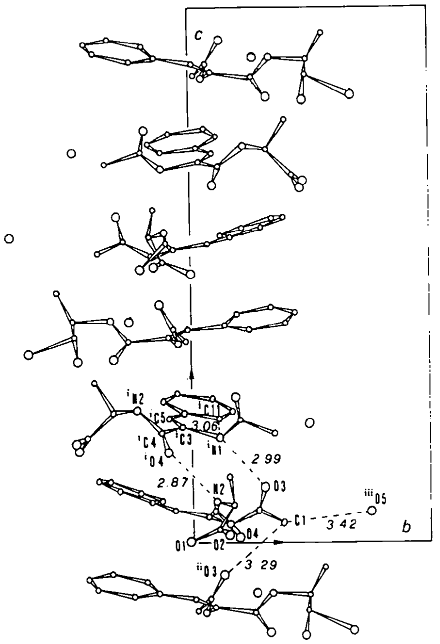

Fig. 2. Crystal packing along the *x* axis. Symmetry code: (i) *y*, *y*−*x*, $\frac{1}{6}+z$; (ii) *x*−*y*, *x*, $z-\frac{1}{6}$; (iii) *x*, *y*+1, *z*; (iv) *x*−1, *y*, *z*; (v) *y*, *y*−*x*+1, $\frac{1}{6}+z$.

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* A preliminary account on this structure has been presented by Busetti, Ajò & Granozzi (1982).

* Lists of structure factors and anisotropic thermal parameters for the non-hydrogen atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39329 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates* ($\times 10^4$, *for* H *atoms* $\times 10^3$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^3$) *with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
O(1)	4686 (6)	−11 (8)	0	80 (3)
O(2)	6806 (7)	2066 (9)	93 (4)	86 (3)
O(3)	1424 (6)	3025 (6)	1079 (4)	64 (2)
O(4)	3259 (5)	2332 (6)	19 (4)	59 (2)
O(5)	2659 (22)	−2560 (23)	672 (10)	
N(1)	435 (6)	1606 (6)	324 (4)	37 (2)
N(2)	3400 (6)	1073 (7)	754 (4)	51 (3)
C(1)	291 (12)	3815 (11)	405 (6)	66 (4)
C(2)	751 (7)	2786 (7)	629 (4)	39 (3)
C(3)	1020 (7)	681 (8)	474 (4)	41 (3)
C(4)	2644 (7)	1422 (7)	396 (4)	43 (3)
C(5)	210 (9)	−709 (8)	622 (4)	53 (3)
C(6)	−1363 (8)	−1634 (8)	728 (5)	50 (3)
C(7)	−1833 (12)	−3018 (10)	936 (6)	91 (5)
C(8)	−3326 (13)	−3927 (12)	1067 (7)	105 (6)
C(9)	−4300 (12)	−3444 (14)	1004 (6)	98 (6)
C(10)	−3831 (13)	−2122 (16)	813 (8)	113 (7)
C(11)	−2366 (11)	−1203 (12)	661 (7)	99 (6)
C(12)	4959 (8)	1733 (9)	706 (4)	49 (3)
C(13)	5631 (13)	1562 (18)	1245 (5)	93 (7)
C(14)	5427 (9)	1136 (9)	228 (4)	55 (4)
H(1,O2)	164 (10)	470 (10)	160 (4)	
H(1,N1)	−16 (8)	137 (8)	0 (3)	
H(1,N2)	290 (8)	48 (8)	102 (3)	
H(1,C1)†	−23	363	6	
H(2,C1)†	116	474	36	
H(3,C1)†	−32	388	69	
H(1′,C1)†	52	466	62	
H(2′,C1)†	−74	327	36	
H(3′,C1)†	74	415	5	
H(1,C5)	74 (7)	876 (8)	65 (3)	
H(1,C12)	538 (8)	277 (8)	64 (3)	
H(1,C13)	530 (8)	61 (8)	125 (4)	
H(2,C13)	663 (9)	199 (8)	130 (3)	
H(3,C13)	535 (9)	198 (8)	150 (3)	
H(1,C7)	−120 (8)	−333 (8)	89 (3)	
H(1,C8)	−377 (8)	−494 (8)	116 (3)	
H(1,C9)	−540 (9)	−410 (8)	112 (3)	
H(1,C10)	−422 (9)	−185 (10)	68 (4)	
H(1,C11)	−221 (8)	−45 (9)	56 (4)	

† Coordinates of the half-occupancy C(1) methyl H atoms, derived from a Fourier difference map, could not be refined, so they are in calculated positions.

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

O(1)–C(14)	1·19 (1)	C(3)–C(5)	1·32 (1)
O(2)–C(14)	1·32 (1)	C(5)–C(6)	1·46 (1)
O(3)–C(2)	1·24 (1)	C(6)–C(7)	1·38 (1)
O(4)–C(4)	1·23 (1)	C(6)–C(11)	1·35 (2)
N(1)–C(2)	1·33 (1)	C(7)–C(8)	1·41 (1)
N(1)–C(3)	1·43 (1)	C(8)–C(9)	1·36 (2)
N(2)–C(4)	1·34 (1)	C(9)–C(10)	1·30 (2)
N(2)–C(12)	1·43 (1)	C(10)–C(11)	1·40 (1)
C(1)–C(2)	1·49 (2)	C(12)–C(13)	1·52 (2)
C(3)–C(4)	1·50 (1)	C(12)–C(14)	1·50 (1)

C(2)–N(1)–C(3)	120·5 (7)	C(5)–C(6)–C(7)	117·0 (9)
C(4)–N(2)–C(12)	120·8 (7)	C(7)–C(6)–C(11)	118·1 (9)
N(1)–C(2)–C(1)	117·7 (8)	C(6)–C(7)–C(8)	119·2 (10)
O(3)–C(2)–C(1)	121·5 (8)	C(7)–C(8)–C(9)	121·0 (10)
O(3)–C(2)–N(1)	120·8 (8)	C(8)–C(9)–C(10)	118·9 (14)
N(1)–C(3)–C(5)	124·1 (8)	C(9)–C(10)–C(11)	121·8 (14)
N(1)–C(3)–C(4)	112·5 (6)	C(6)–C(11)–C(10)	121·0 (11)
C(4)–C(3)–C(5)	123·2 (8)	N(2)–C(12)–C(14)	113·3 (8)
N(2)–C(4)–C(3)	117·5 (7)	N(2)–C(12)–C(13)	111·4 (8)
O(4)–C(4)–C(3)	121·0 (7)	C(13)–C(12)–C(14)	108·6 (9)
O(4)–C(4)–N(2)	121·5 (7)	O(2)–C(14)–C(12)	110·1 (8)
C(3)–C(5)–C(6)	132·2 (8)	O(1)–C(14)–C(12)	125·8 (8)
C(5)–C(6)–C(11)	124·8 (8)	O(1)–C(14)–O(2)	124·1 (8)

Bond angles C(5)–C(6)–C(7) = 117·0 (9) and C(5)–C(6)–C(11) = 124·8 (8)° are significantly different ($\Delta/\sigma = 6{\cdot}5$) and both C(3)–C(5)–C(6) = 132·2 (8) and N(1)–C(3)–C(5) = 124·1 (8)° are larger than the expected 120° value: this may be ascribed to the tendency of the phenyl ring to be coplanar with the C(5)–C(3)–N(1) system.

There is an intramolecular short contact between the C(11) phenyl carbon atom and the acetylamino nitrogen atom: C(11)···N(1) = 3·06 (1), H(C11)···N(1) = 2·59 (7) Å, C(11)–H(C11)···N(1) = 121 (8)°.

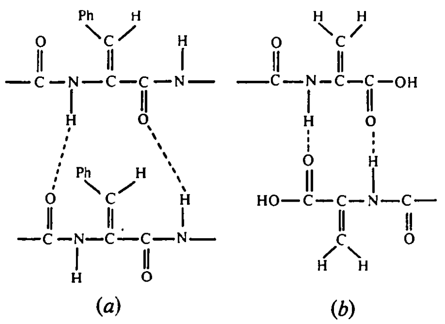
Molecules are arranged in helices along the *z* axis by three intermolecular hydrogen contacts (Å, deg):

$$\mathrm{N(2)\cdots O(4^{i}) = 2{\cdot}87\ (1),\quad H(N2)\cdots O(4^{i}) = 2{\cdot}04\ (7)}$$
$$\mathrm{N(2){-}H(N2)\cdots O(4^{i}) = 161\ (9)}$$
$$\mathrm{O(3)\cdots N(1^{i}) = 2{\cdot}99\ (1),\quad O(3)\cdots H(N1^{i}) = 2{\cdot}08\ (9)}$$
$$\mathrm{O(3)\cdots H(N1^{i}){-}N(1) = 159\ (7)}$$
$$\mathrm{O(3)\cdots C(1^{i}) = 3{\cdot}30\ (1),\quad O(3)\cdots H(1,C1^{i}) = 2{\cdot}6\ (1)}$$
$$\mathrm{O(3)\cdots H(1,C1^{i}){-}C(1^{i}) = 136\ (8).}$$

These helices are held side by side by three hydrogen contacts, all involving the C(1) methyl group:

$$\mathrm{C(1)\cdots O(1^{v}) = 3{\cdot}47\ (1),\quad H(3,C1)\cdots O(1^{v}) = 2{\cdot}72\ (2)}$$
$$\mathrm{C(1){-}H(3,C1)\cdots O(1^{v}) = 138\ (7)}$$
$$\mathrm{C(1)\cdots O(5^{iii}) = 3{\cdot}42\ (2),\quad H(2,C1)\cdots O(5^{iii}) = 2{\cdot}58\ (9)}$$
$$\mathrm{C(1){-}H(2,C1)\cdots O(5^{iii}) = 147\ (9)}$$
$$\mathrm{C(1)\cdots O(2^{iv}) = 3{\cdot}27\ (1),\quad H(2',C1)\cdots O(2^{iv}) = 2{\cdot}33\ (9)}$$
$$\mathrm{C(1){-}H(2',C1)\cdots O(2^{iv}) = 170\ (9).}$$

Molecules are parallel (*a*) as far as the alignment of the amide groups is concerned. This is possible only with non-planar conformation around φ; in fact, the antiparallel (*b*) alignment is preferred for dehydro-Ala-OH which preferentially assumes a planar conformation.



This behaviour is peculiar to all even polyamides (Clark & Wilson, 1973).

Dimensions of the unsaturated peptide unit are to some extent different from those usually found in simple peptides (Marsh & Donohue, 1967).

The conformation of the dehydro-Phe residue is described by the following values of the torsion angles:

$$\omega_1[\mathrm{C(1){-}C(2){-}N(1){-}C(3)}] = 171\ (1),$$
$$\varphi_1[\mathrm{C(2){-}N(1){-}C(3){-}C(4)}] = -68\ (1),$$
$$\psi_1[\mathrm{N(1){-}C(3){-}C(4){-}N(2)}] = 147\ (1),$$
$$\chi_1[\mathrm{N(1){-}C(3){-}C(5){-}C(6)}] = -6\ (2),$$
$$\chi_2[\mathrm{C(3){-}C(5){-}C(6){-}C(7)}] = -173\ (1)°.$$

The conformation of dehydro-Phe-Ala-OH corresponds to the minimum-energy region V in the conformational energy map of the dehydro-Phe residue (Ajò, Casarin & Granozzi, 1982; Ajò, Busetti & Granozzi, 1982; see in particular Fig. 6 in the latter) while that of the corresponding fragment in (dehydro-Phe)$_2$-Ala-OH is related to region II. This difference can be ascribed to the different intermolecular packing; the intramolecular ten-membered ring suggested for doubly unsaturated *N*-acetyltripeptides (Pieroni, Fissi, Merlino & Ciardelli, 1976–77) is obviously impossible for the dipeptide dehydro-Phe-Ala-OH but is also absent in the crystal structure of (dehydro-Phe)$_2$-Ala-OH.

The conformation of the alanine residue is described by the following values of the torsion angles:

ω_2[C(3)—C(4)—N(2)—C(12)] = 180 (1),
φ_2[C(4)—N(2)—C(12)—C(14)] = −75 (1),
ψ_2[N(2)—C(12)—C(14)—O(2)] = 160 (1)°.

This conformation of the alanine residue was described as the preferred one (Nakayama, Maeda, Kaneko & Katsura, 1971) for dehydrophenylalanyl dipeptides in relation to their asymmetric reduction. However, it is different from that of the same residue in (dehydro-Phe)$_2$-Ala.

These results point to a relevant mutual influence between the conformation of unsaturated residues and the nature and conformation of the following saturated one. This further supports our idea that conformational flexibility of unsaturated residues is similar to that of the saturated ones. In fact, previously reported theoretical predictions on this class of compounds is now further corroborated, since experimental conformations correspond to low calculated energy regions, and several predicted minimum-energy regions are populated.

We thank Professor Osvaldo Pieroni and his colleagues for the gift of dehydro-Phe-Ala-OH and for helpful discussions.

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Structure of L-Tyrosyl-L-valine Monohydrate, $C_{14}H_{20}N_2O_4.H_2O$

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Abstract. $M_r = 298{\cdot}34$, orthorhombic, $P2_12_12_1$, $a = 5{\cdot}629\ (1)$, $b = 8{\cdot}702\ (2)$, $c = 31{\cdot}007\ (8)$ Å, $V = 1519\ (1)$ Å^3, $Z = 4$, $D_m = 1{\cdot}31$, $D_x = 1{\cdot}30$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 0{\cdot}737$ mm^{-1}, $F(000) = 640{\cdot}0$, $T = 293$ K, final $R = 0{\cdot}071$ for 1144 unique observed reflections. The crystal structure is stabilized by extensive hydrogen-bonding involving N and O atoms. The molecule exists as a zwitterion with the