Comme pour le R7000, la cohésion cristalline est assurée simultanément par des interactions du type CH···O mettant en jeu les oxygènes des groupes $-NO_2$ et $-OCH_3$ [(*a*) O(22,I)···C(7,I + *a* + *b* + *c*) = 3,33, O(22,I)···H(107,I + *a* + *b* + *c*) = 2,41 Å; (*b*) O(23,I)···C(4,I–*b*) = 3,49, O(23,I)···H(104,I–*b*) = 2,50 Å] et par des interactions résultant du recouvrement des orbitales π de molécules parallèles et superposées (forces de stacking); ces dernières forment un empilement quasi régulier avec des distances interplanaires de 3,33 et 3,37 Å.

La molécule présentement étudiée (R7105) et ses homologues les R7000 et R6998 ne diffèrent apparemment que par leur forme globale. Bien qu'on ne sache pas encore comment agissent ces molécules, les différences d'activité entre ces substances pourraient être dues simultanément à leur géométrie et à la distribution des charges atomiques du noyau naphtofuranne.

Références

Bideau, J.-P., Bravic, G., Cotrait, M. & Courseille, C. (1983). *Acta Cryst.* C**39**, 1101–1103.

Bravic, G., Bideau, J.-P. & Courseille, C. (1982). *Cryst. Struct. Commun.* **11**, 409–412.

Cavier, R., Buisson, J. P., Lemoine, J. & Royer, R. (1981). *Eur. J. Med. Chem.* **16**, 73–76.

Cromer, D. T. & Waber, J. T. (1974). Dans *International Tables for X-ray Crystallography*, Tome IV, édité par J. A. Ibers & W. C. Hamilton. Birmingham: Kynoch Press.

Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

Main, P., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. de York, Angleterre, et de Louvain, Belgique.

Royer, R. & Buisson, J. P. (1980). *Eur. J. Med. Chem.* **2**, 275–278.

Stewart, R. F., Davidson, E. R. & Simpson, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

Weil-Thévenet, N., Buisson, J. P., Royer, R. & Hofnung, M. (1981). *Mutat. Res.* **88**, 355–362.

Acta Cryst. (1984). C**40**, 324–327

Structure of Ethyl (*Z*)-*N*-Acetyldehydrophenylalaninate, $C_{13}H_{15}NO_3$

By D. Ajò

Istituto di Chimica e Tecnologia dei Radioelementi del CNR, Corso Stati Uniti, 35100 *Padova, Italy*

V. Busetti

Istituto di Chimica Organica dell'Università, Via Marzolo 1, 35100 *Padova, Italy*

and H. C. J. Ottenheijm and R. Plate

Department of Organic Chemistry, University of Nijmegen, Toernooiveld, 6525 *ED Nijmegen, The Netherlands*

(*Received* 9 *June* 1983; *accepted* 21 *September* 1983)

Abstract. $M_r = 233{\cdot}26$, orthorhombic, *Pbca*, $a = 49{\cdot}869\,(5)$, $b = 10{\cdot}898\,(2)$, $c = 9{\cdot}544\,(2)$ Å, $V = 5187\,(1)$ Å^3, $Z = 16$, $D_x = 1{\cdot}195$, $D_m = 1{\cdot}18$ Mg m^{-3} (by flotation in aqueous KI solution), μ(Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å) $= 0{\cdot}795$ mm^{-1}, $F(000) = 1984$, $T = 298$ K, $R = 0{\cdot}095$ for 1758 reflections with $I > 2{\cdot}5\sigma(I)$. There are two independent molecules in a unit cell. They are approximate enantiomers ($\varphi = 80{\cdot}8°$ for molecule *A* and $-64{\cdot}0°$ for *B*).

Introduction. Many biologically important peptides contain α, β-unsaturated amino acid residues which are particularly interesting because of their unusual conformational (Ajò, Granozzi, Tondello & Del Pra, 1980, and references therein; Ajò, Casarin & Granozzi, 1982; Ajò, Busetti & Granozzi, 1982; Busetti, Ajò & Granozzi, 1982) and electronic (Ajò, Granozzi, Ciliberto & Fragalà, 1980; Ajò, Casarin, Granozzi & Busetti, 1981) 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).

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

Conformational studies of dehydrophenylalanine and its derivatives are of interest not only from a biological point of view (Rich & Bhatnagar, 1978, and references

0108-2701/84/020324-04$01.50

therein; Ajò, Granozzi, Tondello & Del Pra, 1980) but also in order to investigate the 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).

Experimental. Preparation of title compound reported previously (Herscheid, Scholten, Tijhuis & Ottenheijm, 1981). Needle-shaped crystal 0·20 x 0·20 x 1·20 mm. Philips PW 1100 four-circle diffractometer, Mo $K\alpha$ radiation monochromatized by a graphite plate, θ–2θ scan mode, scan width 1·4°, scan speed 0·035° s^{-1}, background measured for 7 s at each extremity, θ 2 to 25°. Two standard intensity and orientation reflections (12,0,0 and $\overline{12}$,0,0) measured at 3 h intervals: no significant variation. Unit cell: least-squares refinement of θ values of 32 high-angle reflections. 4369 measured reflections, 1758 observed [$I > 2{\cdot}5\sigma(I)$]. Lorentz–polarization correction, no absorption correction. Structure solved by direct methods; E map revealed positions of all non-hydrogen atoms; subsequent difference Fourier synthesis gave positions of H atoms. Full-matrix least-squares refinement (on F), anisotropic temperature factors for non-hydrogen atoms, unit weights, $(\Delta/\sigma)_{mean}$ 0·03. For H atoms only positional parameters refined; thermal parameters, from the bonded atoms, held constant. Final difference map revealed no peak >0·36 e Å^{-3}. No correction for secondary extinction. 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-OEt) (with the numbering of the atoms and the nomenclature of relevant torsion angles) is reported in Fig. 1, and final positional parameters are in Table 1.[*] From U_{eq} values of C(12), C(13) and C(13′) some disorder is evident in the ethyl groups. Bond distances and angles are shown in Table 2, and the crystal packing is given in Fig. 2. Short contacts have been detected between molecules at the origin and those at $x, \frac{1}{2}-y, \frac{1}{2}+z$ [N(1)···O(3^{i}) 2·856 (6), N(1′)···O(3′^{i}) 2·797 (5) Å; N(1)–H(1,N1)···O(3^{i}) 177 (5), N(1′)–H(1,N1′)···O(3′^{i}) 138 (5)°].

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

Unprimed atoms correspond to molecule *A*, primed atoms to molecule *B*.

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

	x	y	z	U_{eq}
O(1)	7360 (1)	443 (4)	4740 (5)	82 (2)
O(2)	7067 (1)	−978 (4)	4007 (4)	72 (2)
O(3)	6980 (1)	2884 (4)	3879 (4)	75 (2)
N(1)	6977 (1)	1861 (6)	5901 (5)	49 (2)
C(1)	7066 (2)	4002 (6)	5970 (7)	69 (3)
C(2)	7007 (1)	2895 (7)	5172 (7)	43 (3)
C(3)	6910 (1)	726 (6)	5279 (6)	41 (3)
C(4)	7135 (1)	65 (7)	4637 (6)	62 (3)
C(5)	6661 (2)	296 (6)	5272 (6)	54 (3)
C(6)	6410 (1)	775 (6)	5823 (6)	44 (3)
C(7)	6388 (1)	1726 (6)	6856 (7)	55 (3)
C(8)	6142 (2)	2088 (6)	7336 (7)	63 (3)
C(9)	5913 (2)	1564 (7)	6863 (8)	66 (4)
C(10)	5924 (2)	661 (8)	5860 (8)	64 (3)
C(11)	6171 (2)	255 (6)	5390 (7)	57 (3)
C(12)	7279 (1)	−1694 (8)	3405 (9)	94 (4)
C(13)	7177 (2)	−2748 (9)	2632 (9)	126 (5)
O(1′)	4901 (1)	4650 (4)	2040 (4)	64 (2)
O(2′)	4615 (1)	6192 (3)	1598 (4)	47 (2)
O(3′)	4496 (1)	3014 (4)	166 (3)	59 (2)
N(1′)	4459 (1)	3085 (4)	2525 (4)	45 (2)
C(1′)	4537 (1)	1104 (6)	1440 (7)	54 (3)
C(2′)	4499 (1)	2469 (6)	1302 (6)	44 (2)
C(3′)	4433 (2)	4373 (5)	2518 (6)	39 (3)
C(4′)	4674 (1)	5046 (5)	2050 (6)	38 (2)
C(5′)	4218 (1)	4928 (5)	3044 (6)	44 (3)
C(6′)	3972 (1)	4355 (6)	3589 (5)	44 (3)
C(7′)	3826 (2)	4949 (7)	4658 (7)	64 (3)
C(8′)	3599 (2)	4448 (9)	5185 (8)	81 (4)
C(9′)	3497 (2)	3390 (9)	4639 (9)	78 (4)
C(10′)	3630 (2)	2834 (7)	3541 (8)	71 (4)
C(11′)	3866 (2)	3313 (7)	3035 (7)	55 (3)
C(12′)	4841 (2)	6913 (7)	1074 (7)	68 (4)
C(13′)	4726 (2)	7928 (7)	257 (8)	95 (4)

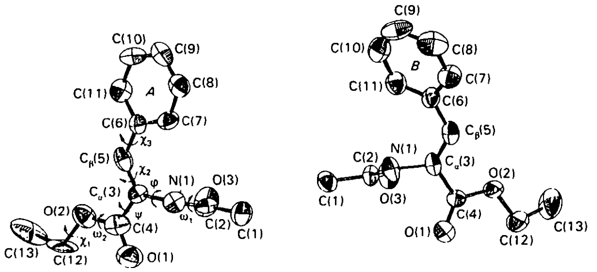

Fig. 1. *ORTEP*II projection of dehydro-Phe-OEt viewed along the *c* axis.

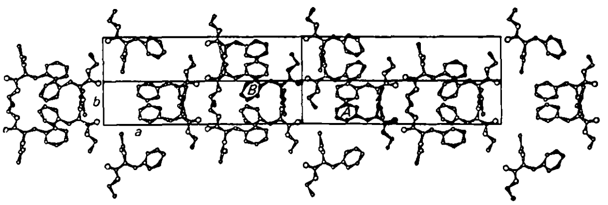

Fig. 2. The crystal packing projected along the *c* axis.

---

[*] Lists of structure factors, H-atom parameters and anisotropic thermal parameters for non-hydrogen atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38888 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

	A	*B*		*A*	*B*
O(1)—C(4)	1·199 (7)	1·211 (7)	C(4)—O(2)—C(12)	117·3 (4)	115·9 (4)
O(2)—C(4)	1·330 (8)	1·354 (6)	C(2)—N(1)—C(3)	123·2 (5)	120·0 (5)
O(2)—C(12)	1·434 (8)	1·462 (8)	N(1)—C(2)—C(1)	116·7 (6)	115·5 (5)
O(3)—C(2)	1·241 (8)	1·236 (7)	O(3)—C(2)—C(1)	123·3 (6)	123·6 (5)
N(1)—C(2)	1·333 (9)	1·361 (7)	N(1)—C(3)—C(5)	122·2 (6)	121·7 (5)
N(1)—C(3)	1·412 (9)	1·410 (7)	N(1)—C(3)—C(4)	115·1 (5)	114·9 (5)
C(1)—C(2)	1·457 (9)	1·505 (9)	C(4)—C(3)—C(5)	122·7 (6)	123·0 (5)
C(3)—C(4)	1·467 (8)	1·477 (10)	O(2)—C(4)—C(3)	114·4 (5)	112·2 (5)
C(3)—C(5)	1·327 (11)	1·329 (10)	O(1)—C(4)—C(3)	120·8 (6)	125·9 (5)
C(5)—C(6)	1·455 (10)	1·472 (8)	O(1)—C(4)—O(2)	124·7 (5)	122·0 (5)
C(6)—C(7)	1·435 (9)	1·411 (10)	C(3)—C(5)—C(6)	132·6 (6)	127·8 (5)
C(6)—C(11)	1·383 (11)	1·360 (10)	C(5)—C(6)—C(11)	119·1 (6)	122·8 (6)
C(7)—C(8)	1·368 (11)	1·354 (13)	C(5)—C(6)—C(7)	125·0 (5)	119·4 (6)
C(8)—C(9)	1·354 (13)	1·364 (14)	C(7)—C(6)—C(11)	115·8 (6)	117·6 (6)
C(9)—C(10)	1·374 (11)	1·380 (12)	C(6)—C(7)—C(8)	120·5 (6)	121·0 (7)
C(10)—C(11)	1·384 (13)	1·375 (13)	C(7)—C(8)—C(9)	121·5 (7)	120·7 (8)
C(12)—C(13)	1·457 (13)	1·470 (11)	C(8)—C(9)—C(10)	120·0 (9)	118·8 (9)
			C(9)—C(10)—C(11)	119·4 (8)	120·8 (8)
			C(6)—C(11)—C(10)	122·6 (7)	120·9 (7)
			O(2)—C(12)—C(13)	112·0 (6)	106·6 (5)

Table 3. *Values of relevant torsion angles* (°)

	Molecule *A*	Molecule *B*
ω_1 [C(1)—C(2)—N(1)—C(3)]	177·7 (6)	177·2 (5)
φ [C(2)—N(1)—C(3)—C(4)]	80·8 (7)	−64·0 (8)
ψ [N(1)—C(3)—C(4)—O(2)]	−177·4 (5)	158·5 (5)
ω_2 [C(3)—C(4)—O(2)—C(12)]	−177·6 (5)	−178·2 (5)
χ_1 [C(4)—O(2)—C(12)—C(13)]	−174·4 (6)	162·8 (5)
χ_2 [N(1)—C(3)—C(5)—C(6)]	0·(1)	−5·(1)
χ_3 [C(3)—C(5)—C(6)—C(7)]	−18·(1)	150·2 (7)

Dimensions of the peptide group are to some extent different from those usually found in simple peptides (Marsh & Donohue, 1967). Also, comparison with analogous systems gives contradictory results: in particular, the N—C$_\alpha$ bond length [1·412 (9) Å in molecule *A* and 1·410 (7) Å in molecule *B*] is similar to the reported ones for both dehydro-Ala-OH [1·409 (5) Å] and dehydro-Pro-OH [1·416 (5) Å], but is shorter than that of dehydro-Phe-OH [1·438 (6) Å].

Conformations of the two independent molecules in the asymmetric unit are described in Table 3 and both are located in the minimum-energy region IV in the conformational-energy map of dehydro-Phe-OH (Ajò, Casarin, Granozzi & Busetti, 1981). Molecules *A* and *B* are approximate enantiomers ($\varphi = 80{\cdot}8°$ for molecule *A* and $\varphi = -64{\cdot}0°$ for molecule *B*).

The main difference between these results and those of dehydro-Phe-OH is represented by the *transoid* conformation as far as ψ is concerned, while a *cisoid* conformation is assumed by the corresponding carboxylic acid (Ajò, Casarin, Granozzi & Busetti, 1981).

This is in line with results of *N*-acetyl-2,3-didehydroproline (dehydro-Pro-OH) (Ajò, Busetti, Granozzi & Liakopoulou-Kyriakides, 1984) which is *cisoid* as far as torsion angle ψ is concerned [to be compared with the corresponding *transoid* esterified fragment in virginiamycin (Durant, Evrard, Declercq & Germain, 1974)], and it supports a relevant role of intermolecular (in particular, hydrogen-bonding) interactions. On the other hand, even if only esterified systems are taken into account, different conformations are possible in different environments: for instance, dehydro-Phe-OMe assumes a *transoid* conformation as far as ψ is concerned both in Fe(CO)$_3$ (De Cian, Weiss, Haudegond, Chauvin & Commereuc, 1980) and [Rh(diphos)]$^+$ (Chan, Pluth & Halpern, 1979) complexes, while dehydro-Phe-OEt is *cisoid* in the analogous [Rh(*S*,*S*-chiraphos)]$^+$ complex (Chan, Pluth & Halpern, 1980).* Finally, it is noteworthy that different conformations are assumed by the ester alkyl group in the title compound (*trans*) and in the corresponding Rh complex (*gauche*). It must be noted that the metal coordination is quite similar (through both the amide O atom and the C=C group) in all three above-quoted metal complexes.

---

* diphos = $(C_6H_5)_2PCH_2CH_2P(C_6H_5)_2$; chiraphos = $(C_6H_5)_2PCHCH_3CHCH_3P(C_6H_5)_2$.

References

Achiwa, K., Chaloner, P. A. & Parker, D. (1981). *J. Organomet. Chem.* **218**, 249–260.

Ajò, D., Busetti, V. & Granozzi, G. (1982). *Tetrahedron*, **38**, 3329–3334.

Ajò, D., Busetti, V., Granozzi, G. & Liakopoulou-Kyriakides, M. (1984). *Acta Cryst.* C**40**, 327–330.

Ajò, D., Casarin, M. & Granozzi, G. (1982). *J. Mol. Struct.* **86**, 297–300.

Ajò, D., Casarin, M., Granozzi, G. & Busetti, V. (1981). *Tetrahedron*, **37**, 3507–3512.

Ajò, D., Granozzi, G., Ciliberto, E. & Fragalà, I. (1980). *J. Chem. Soc. Perkin Trans.* 2, pp. 483–485.

Ajò, D., Granozzi, G., Tondello, E. & Del Pra, A. (1980). *Biopolymers*, **19**, 469–475.

Ajò, D., Granozzi, G., Tondello, E., Del Pra, A. & Zanotti, G. (1979). *J. Chem. Soc. Perkin Trans.* 2, pp. 927–929.

Bacciola, D., Balestreri, E., Felicioli, R. A., Fissi, A. & Pieroni, O. (1976). *Chim. Ind.* (*Milan*), **58**, 519.

Busetti, V., Ajò, D. & Granozzi, G. (1982). Abstr. Seventh Eur. Crystallogr. Meet. (Jerusalem), 188.

Chan, A. S. C., Pluth, J. J. & Halpern, J. (1979). *Inorg. Chim. Acta*, **37**, L477–L479.

Chan, A. S. C., Pluth, J. J. & Halpern, J. (1980). *J. Am. Chem. Soc.* **102**, 5952–5954.

De Cian, A., Weiss, R., Haudegond, J.-P., Chauvin, Y. & Commereuc, D. (1980). *J. Organomet. Chem.* **187**, 73–80.

Durant, F., Evrard, G., Declercq, J.-P. & Germain, G. (1974). *Cryst. Struct. Commun.* pp. 503–510.

Herscheid, J. D. M., Scholten, H. P. H., Tijhuis, M. W. & Ottenheijm, H. C. J. (1981). *Recl Trav. Chim. Pays-Bas*, **97**, 73–78.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee.

Main, P., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

MARSH, R. E. & DONOHUE, J. (1967). *Adv. Protein Chem.* **22**, 235–256.

NAKAYAMA, M., MAEDA, G., KANEKO, T. & KATSURA, H. (1971). *Bull. Chem. Soc. Jpn*, **44**, 1150–1152.

RICH, D. H. & BHATNAGAR, P. K. (1978). *J. Am. Chem. Soc.* **100**, 2218–2224.

RICH, D. H. & JASENSKY, R. D. (1979). *J. Am. Chem. Soc.* **101**, 5412–5414.

SHELDRICK, G. M. (1976). *SHELX*. Program for crystal structure determination. Univ. of Cambridge, England.

SINOU, D., LAFONT, D., DESCOTES, G. & KENT, A. G. (1981). *J. Organomet. Chem.* **217**, 119–127.

Acta Cryst. (1984). C**40**, 327–330

Structure of *N*-Acetyl-2,3-didehydroproline, $C_7H_9NO_3$

BY D. AJÒ

Istituto di Chimica e Tecnologia dei Radioelementi del CNR, Corso Stati Uniti, 35100 *Padova, Italy*

V. BUSETTI

Istituto di Chimica Organica dell'Università, Via Marzolo 1, 35100 *Padova, Italy*

G. GRANOZZI

Istituto di Chimica Generale ed Inorganica dell'Università, Via Loredan 4, 35100 *Padova, Italy*

AND M. LIAKOPOULOU-KYRIAKIDES

Department of Chemical Engineering of the Aristotle University, Thessaloniki, Greece

(*Received* 4 *July* 1983; *accepted* 21 *September* 1983)

Abstract. $M_r = 155\cdot18$, orthorhombic, *Pbca*, $a = 13\cdot455$ (4), $b = 13\cdot466$ (4), $c = 8\cdot069$ (3)Å, $Z = 8$, $V = 1462\cdot0$ (8) Å^3, $D_x = 1\cdot410$, $D_m = 1\cdot41$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0\cdot90$ mm^{-1}, $F(000) = 656$, $T = 298$ K, final $R = 0\cdot042$ for 625 unique reflections. The molecules exhibit a non-planar conformation and are linked by hydrogen bonds to form one-dimensional chains. The conformational flexibility of this molecular system is discussed also on the basis of the known structures of related compounds and previously reported spectroscopic and theoretical results.

Introduction. α, β-Unsaturated amino acid residues are present in many natural peptides which exhibit biological activities (Rich & Bhatnagar, 1978, and references therein; Ajò, Granozzi, Tondello & Del Pra, 1980, and references therein). They are particularly interesting because of their unusual conformational (Ajò, Granozzi, Tondello & Del Pra, 1980; Ajò, Busetti & Granozzi, 1982; Ajò, Casarin & Granozzi, 1982; Busetti, Ajò & Granozzi, 1982; Ajò, Busetti, Ottenheijm & Plate, 1984) and electronic (Ajò, Granozzi, Ciliberto & Fragalà, 1980; Ajò, Casarin, Granozzi & Busetti, 1981) features.

In previous papers we reported on the crystal and molecular structure of *N*-acetyldehydroalanine (dehydro-Ala-OH) which assumes an extended conformation in the crystal state (Ajò, Granozzi, Tondello, Del Pra & Zanotti, 1979). 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).

These results encouraged us in pursuing conformational investigations of this series of compounds; *N*-acetyl-2,3-didehydroproline (dehydro-Pro-OH) could be of relevant interest, since the presence of a five-membered ring (φ *cisoid*) prevents both conformations found for dehydro-Ala-OH (φ *trans*) and dehydro-Phe-OH (φ = 71·7°).

Conformational studies on dehydro-Pro-OH and suitable derivatives are also of interest in relation to *s-cis–s-trans* isomerization behaviour in solution, which is different both from that of other acylproline analogues and from that of some *N*-substituted α,β-unsaturated acylamino acids (Galardy, Alger & Liakopoulou-Kyriakides, 1982).

Experimental. Crystals of $C_7H_9NO_3$ provided by M. Liakopoulou-Kyriakides (Galardy, Alger & Liakopoulou-Kyriakides, 1982). D_m measured by flotation. Crystal 0·5 × 0·4 × 0·6 mm. Philips PW 1100 four-circle diffractometer. Cell dimensions from 32 high-angle reflections. θ–2θ scan mode, $2 < \theta < 23°$,

0108-2701/84/020327-04$01.50