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N-(3,4-Dichlorophenyl)cyclopropanecarboxamide and *N*-(3,4-Dichlorophenyl)acetamide

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Abstract. $C_{10}H_9Cl_2NO$ (1), $M_r = 230{\cdot}10$, monoclinic, $P2_1/c$, $a = 5{\cdot}025$ (1), $b = 22{\cdot}051$ (5), $c = 9{\cdot}615$ (2) Å, $\beta = 101{\cdot}53$ (2)°, $V = 1044{\cdot}0$ Å^3, $Z = 4$, $D_x = 1{\cdot}46$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}6$ mm^{-1}, $F(000) = 472$, $T = 293$ K. The structure was refined to $R = 0{\cdot}038$ for 1525 unique observed reflections. $C_8H_7Cl_2NO$ (2), $M_r = 204{\cdot}05$, triclinic, $P\bar{1}$, $a = 7{\cdot}254$ (2), $b = 9{\cdot}848$ (2), $c = 13{\cdot}441$ (3) Å, $\alpha = 90{\cdot}86$ (2), $\beta = 99{\cdot}78$ (2), $\gamma = 103{\cdot}61$ (2)°, $V = 917{\cdot}9$ Å^3, $Z = 4$, $D_x = 1{\cdot}48$ Mg m^{-3}, $\mu = 0{\cdot}7$ mm^{-1}, $F(000) = 416$, $T = 293$ K. The structure was refined to R 0·047 for 2930 unique observed reflections. In (1) the N—H bond is *syn* to the *meta*-Cl substituent, whereas in both independent molecules of (2) the conformation is *anti*. The C—N—C bond angles are wide (127–129°), consistent with a known correlation with the dihedral angle between phenyl and amide planes and attributable to steric interactions between the O atom and H(2), the *ortho* H atom. In both

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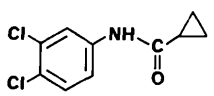
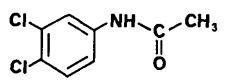
compounds the molecules are linked in chains by N—H···O hydrogen bonding.

Introduction. We have recently observed by NMR methods (Camilleri, Kirby, Lewis & Sanders, 1988) that anilides show a measurable preference for the conformation with N—H *anti* to an electron-withdrawing *meta* substituent. The analysis of the crystal structures of (1) and (2) was intended to show whether this preference is mirrored in the solid state.



(1)



(2)

Experimental. Both compounds were prepared by standard methods. Single crystals were grown by vapour diffusion of petroleum ether into solutions in ethyl acetate.

Compound (1): A colourless block 0·7 × 0·55 × 0·35 mm was mounted in a glass capillary. 1833 profile-fitted intensities (Clegg, 1981) were recorded on a Stoe–Siemens four-circle diffractometer using monochromated Mo $K\alpha$ radiation ($2\theta_{max}$ 50°, ω scans). Three check reflections showed no significant intensity change. No absorption correction. Merging equivalents gave 1827 unique reflections (index ranges after merging h −5 to 5, k 0 to 25, l 0 to 11), of which 1525 with $F > 4\sigma(F)$ were used for all calculations *via* program system *SHELX*76 (Sheldrick, 1976) modified by its author. Cell constants were refined from 2θ values of 52 reflections in the range 20–23°.

The structure was solved by routine direct methods and subjected to full-matrix anisotropic least-squares refinement on F. H atoms were identified in difference syntheses and refined freely. The final R value was 0·038, with wR 0·048. The weighting scheme was $w^{-1} = \sigma^2(F) + 0{\cdot}0002F^2$. 163 parameters; S 2·1; max. Δ/σ 0·003; max. $|\Delta\rho|$ 0·3 e Å^{-3} near Cl(2). Atomic scattering factors were those incorporated in *SHELX*76. Final atomic coordinates are presented in Table 1(*a*),* with derived bond lengths and angles in Table 2(*a*). The molecule is shown in Fig. 1.

Compound (2): as for (1), with the following differences. Crystal size 0·8 × 0·6 × 0·3 mm (colourless prism); ω/θ scans, 4974 reflections, 3228 unique (R_{int} 0·014), 2930 observed (index ranges after merging h −8 to 8, k −11 to 11, l 0 to 15); cell constants refined from 44 reflections in the range 20–22°. H atoms refined freely except for rigid methyl groups with C—H 0·96 Å, H—C—H 109·5°. Final R value 0·047, with wR 0·066; weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}00015F^2$; 255 parameters; S 3·9; max. Δ/σ 0·03; max. $|\Delta\rho|$ 0·6 e Å^{-3} near Cl(1). Final atomic coordinates are given in Table 1(*b*) with derived bond lengths and angles in Table 2(*b*). The two independent molecules are shown in Fig. 2.

Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic displacement parameters* (Å^2 × 10^3)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
(*a*) Compound (1)				
Cl(1)	2284 (1)	4413 (1)	4891 (1)	67 (1)
Cl(2)	2453 (2)	5054 (1)	1959 (1)	86 (1)
C(1)	7439 (4)	3376 (1)	3308 (2)	43 (1)
C(2)	5786 (4)	3612 (1)	4167 (2)	46 (1)
C(3)	4256 (4)	4125 (1)	3772 (2)	49 (1)
C(4)	4353 (5)	4409 (1)	2494 (2)	56 (1)
C(5)	6001 (5)	4174 (1)	1640 (2)	61 (1)
C(6)	7519 (5)	3668 (1)	2027 (2)	55 (1)
N(1)	9082 (4)	2876 (1)	3809 (2)	46 (1)
C(7)	10103 (5)	2458 (1)	3026 (2)	46 (1)
O(1)	9617 (4)	2464 (1)	1727 (1)	67 (1)
C(8)	11819 (5)	1991 (1)	3856 (2)	50 (1)
C(9)	14023 (6)	1711 (1)	3216 (3)	71 (1)
C(10)	11620 (6)	1354 (1)	3281 (4)	73 (1)
(*b*) Compound (2)				
Cl(1)	742 (2)	1690 (1)	10326 (1)	95 (1)
Cl(2)	1600 (1)	4074 (1)	12053 (1)	66 (1)
C(1)	2769 (3)	5075 (2)	8922 (2)	43 (1)
C(2)	2029 (4)	3711 (2)	9139 (2)	51 (1)
C(3)	1681 (4)	3419 (2)	10093 (2)	51 (1)
C(4)	2040 (3)	4457 (2)	10852 (2)	47 (1)
C(5)	2739 (4)	5820 (2)	10625 (2)	54 (1)
C(6)	3103 (4)	6132 (2)	9672 (2)	50 (1)
N	3140 (3)	5442 (2)	7953 (2)	48 (1)
C(7)	3407 (4)	4590 (2)	7215 (2)	51 (1)
O	3375 (3)	3354 (2)	7315 (1)	66 (1)
C(8)	3746 (6)	5273 (3)	6251 (2)	72 (1)
Cl(1′)	2070 (2)	7005 (1)	3667 (1)	90 (1)
Cl(2′)	1354 (1)	9464 (1)	2305 (1)	80 (1)
C(1′)	2798 (3)	10145 (2)	5702 (2)	44 (1)
C(2′)	2657 (4)	8845 (2)	5250 (2)	50 (1)
C(3′)	2203 (4)	8646 (3)	4209 (2)	53 (1)
C(4′)	1915 (4)	9713 (3)	3611 (2)	54 (1)
C(5′)	2068 (4)	11017 (3)	4062 (2)	62 (1)
C(6′)	2503 (4)	11222 (3)	5093 (2)	55 (1)
N′	3245 (3)	10435 (2)	6756 (2)	48 (1)
C(7′)	3453 (4)	9556 (2)	7499 (2)	48 (1)
O′	3316 (3)	8309 (2)	7340 (1)	71 (1)
C(8′)	3923 (5)	10217 (3)	8559 (2)	62 (1)

Discussion. In the crystal structure of (1) (Fig. 1) the *meta*-Cl is *syn* to the N—H bond, contrary to our previous findings; in both molecules of (2) the expected *anti* conformation is observed (Fig. 2). The energy difference between the *syn* and *anti* conformations is small (*ca* 1 kJ mol^{-1}) and would not be expected to determine the solid-state conformation in every case; of 16 anilides in the Cambridge Structural Database (January 1989 version, see Allen, Kennard & Taylor, 1983) or taken from our own work (including the present structures), 13 showed the *anti* conformation (Camilleri *et al.*, 1988).

The two independent molecules of (2) differ somewhat in the torsion angles to the amide side chains

* Lists of structure factors, anisotropic thermal parameters, torsion angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52170 (24 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* (°)

(*a*) Compound (1)

Cl(1)—C(3)	1·722 (2)	Cl(2)—C(4)	1·733 (2)
C(1)—C(2)	1·385 (3)	C(1)—C(6)	1·398 (3)
C(1)—N(1)	1·403 (3)	C(2)—C(3)	1·379 (3)
C(3)—C(4)	1·388 (3)	C(4)—C(5)	1·378 (4)
C(5)—C(6)	1·361 (4)	N(1)—C(7)	1·354 (3)
C(7)—O(1)	1·224 (2)	C(7)—C(8)	1·473 (3)
C(8)—C(9)	1·503 (4)	C(8)—C(10)	1·505 (4)
C(9)—C(10)	1·454 (4)		
C(2)—C(1)—C(6)	118·6 (2)	C(2)—C(1)—N(1)	118·2 (2)
C(6)—C(1)—N(1)	123·1 (2)	C(1)—C(2)—C(3)	120·8 (2)
Cl(1)—C(3)—C(2)	119·3 (2)	Cl(1)—C(3)—C(4)	120·9 (2)
C(2)—C(3)—C(4)	119·8 (2)	Cl(2)—C(4)—C(3)	121·2 (2)
Cl(2)—C(4)—C(5)	119·5 (2)	C(3)—C(4)—C(5)	119·3 (2)
C(4)—C(5)—C(6)	121·1 (2)	C(1)—C(6)—C(5)	120·3 (2)
C(1)—N(1)—C(7)	127·3 (2)	N(1)—C(7)—O(1)	122·7 (2)
N(1)—C(7)—C(8)	114·9 (2)	O(1)—C(7)—C(8)	122·4 (2)
C(7)—C(8)—C(9)	117·7 (2)	C(7)—C(8)—C(10)	117·7 (2)
C(9)—C(8)—C(10)	57·8 (2)	C(8)—C(9)—C(10)	61·2 (2)
C(8)—C(10)—C(9)	61·0 (2)		

(*b*) Compound (2)

	Molecule (I)	Molecule (II)		Molecule (I)	Molecule (II)
Cl(1)—C(3)	1·734 (2)	1·737 (3)	Cl(2)—C(4)	1·729 (2)	1·732 (3)
C(1)—C(2)	1·379 (3)	1·383 (3)	C(1)—C(6)	1·387 (3)	1·383 (3)
C(1)—N	1·411 (3)	1·407 (3)	C(2)—C(3)	1·370 (4)	1·381 (3)
C(3)—C(4)	1·380 (3)	1·366 (4)	C(4)—C(5)	1·378 (3)	1·383 (4)
C(5)—C(6)	1·376 (4)	1·368 (4)	N—C(7)	1·358 (3)	1·343 (3)
C(7)—O	1·221 (3)	1·221 (3)	C(7)—C(8)	1·499 (4)	1·507 (3)
C(2)—C(1)—C(6)	119·1 (2)	118·8 (2)	C(2)—C(1)—N	122·3 (2)	123·2 (2)
C(6)—C(1)—N	118·5 (2)	118·0 (2)	C(1)—C(2)—C(3)	119·7 (2)	119·6 (2)
Cl(1)—C(3)—C(2)	117·9 (2)	118·3 (2)	Cl(1)—C(3)—C(4)	120·2 (2)	120·3 (2)
C(2)—C(3)—C(4)	121·9 (2)	121·4 (2)	Cl(2)—C(4)—C(3)	121·4 (2)	121·4 (2)
Cl(2)—C(4)—C(5)	120·4 (2)	119·6 (2)	C(3)—C(4)—C(5)	118·2 (2)	119·1 (2)
C(4)—C(5)—C(6)	120·7 (2)	120·0 (3)	C(1)—C(6)—C(5)	120·4 (2)	121·2 (2)
C(1)—N—C(7)	127·1 (2)	129·2 (2)	N—C(7)—O	123·3 (2)	123·2 (2)
N—C(7)—C(8)	115·1 (2)	115·5 (2)	O—C(7)—C(8)	121·6 (3)	121·3 (2)

[C(2)—C(1)—N—C(7) −21·2 (4), −6·0 (4)°] but are otherwise very similar to each other; the largest difference in bond length is observed for C(7)—N [1·358 (3), 1·343 (3) Å], and in bond angle for C(1)—N—C(7) [127·1 (2), 129·2 (2)°]. The large values of these formally sp^2 bond angles may be due to steric interactions between the O atom and H(2). Chakrabarti & Dunitz (1982) have shown, by analysis of a large number of crystal structures, that there is good negative correlation between this angle and the corresponding torsion angle between the amide and phenyl planes; when the torsion angle is large enough, the bond angle approaches the ideal sp^2 angle 120°. The molecule of (1) shows a similarly wide angle [C(1)—N(1)—C(7) 127·3 (2)°] despite a somewhat larger corresponding torsion angle [C(2)—C(1)—N(1)—C(7) 155·0 (2)°].

Both compounds form hydrogen bonds of the form N—H···O. In (1) the molecules are linked into chains parallel to the *z* axis, with O(1)···H(1) 2·05 (3), O(1)···N(1) 2·865 (5) Å (second atoms at x, $0{\cdot}5-y$, $-0{\cdot}5+z$) (Fig. 3). In (2) similar chains are formed, but parallel to the *y* axis, with O′···H(0) 2·15 (3), O′···N 2·933 (5) Å (second atoms at x, y, z) and O···H(0′) 2·23 (3), O···N′ 2·936 (5) Å (second atoms at x, $-1+y$, z) (Fig. 4). *p*-Chloroacetanilide also displays such hydrogen-bonded chains, with N···O 2·83 Å (Subramanian, 1966).

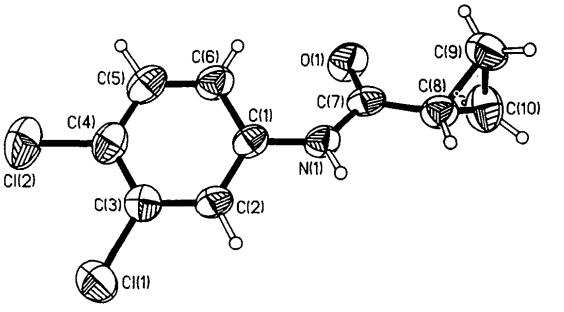


Fig. 1. Thermal-ellipsoid plot (50% level) of the molecule of (1), showing the atom-numbering scheme. H-atom radii are arbitrary.

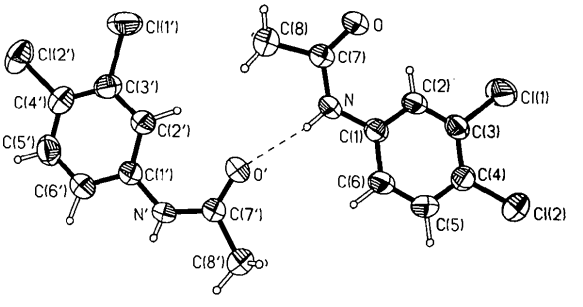


Fig. 2. Thermal-ellipsoid plot (50% level) of the two molecules of (2), showing the atom-numbering scheme. H-atom radii are arbitrary. The hydrogen bond is represented by a dashed line.

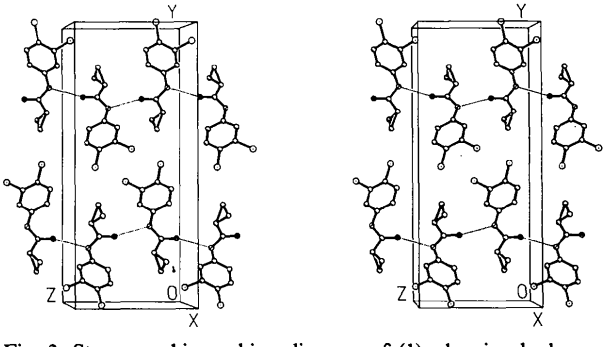


Fig. 3. Stereographic packing diagram of (1), showing hydrogen bonds as dotted lines. Radii are arbitrary; H atoms omitted for clarity.

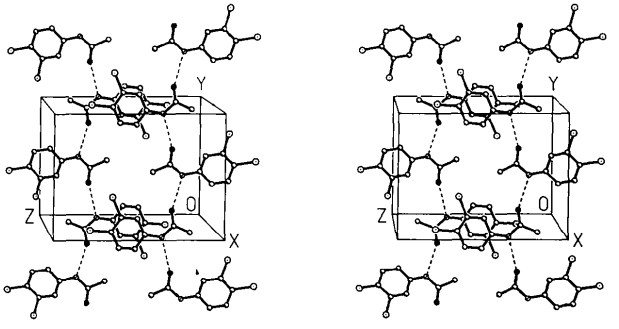


Fig. 4. Stereographic packing diagram of (2), showing hydrogen bonds as dashed lines. Radii are arbitrary. H atoms omitted for clarity.

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Structure of Benzyloxycarbonyl-L-alanyl-L-proline

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Abstract. $C_{16}H_{20}N_2O_5$, $M_r = 320{\cdot}34$, orthorhombic, $P2_12_12_1$, $a = 8{\cdot}503\ (3)$, $b = 22{\cdot}156\ (6)$, $c = 8{\cdot}588\ (3)$ Å, $V = 1617{\cdot}9$ Å^3, $Z = 4$, $D_m = 1{\cdot}30$, $D_x = 1{\cdot}315$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}7107$ Å, $\mu = 0{\cdot}9$ cm^{-1}, $F(000) = 680$, room temperature, $R = 0{\cdot}057$, $wR = 0{\cdot}058$ for 1511 unique reflections [$I > 3\sigma(I)$]. The peptide linkage is in the *trans* conformation. The pyrrolidine ring exists in the envelope conformation. The crystal structure is stabilized by a three-dimensional network of N—H···O and O—H···O hydrogen bonds. There is a stacking interaction between the phenyl group of the benzyloxycarbonyl moiety and the pyrrolidine ring system of the prolyl residue.

Introduction. Proline, a unique imino acid, is an important constituent of many proteins. The five-membered pyrrolidine ring system of proline is formed when the side chain curls back to the protein main chain. This imposes certain restrictions on the conformation of proteins (Balasubramanian, Lakshminarayanan, Sabesan, Tegoni, Venkatesan & Ramachandran, 1971; Ashida & Kakudo, 1974). The conformational aspects of the pyrrolidine ring system are of particular interest as they reveal different modes of puckering in the five-membered ring system (Chacko, Swaminathan & Veena, 1983). In this context the crystal structures of several dipeptides of the type L-Pro-L-*X*, where *X* is one of Gly, Val, Ile, Tyr (reported from this laboratory), Ala, Met and Leu have been found to have similar unit-cell packing, hydrogen bonding and conformation. It seems as though the presence of proline at the N-terminal in these dipeptides dictates the overall conformation irrespective of the second residue. This prompted us to find out whether proline is capable of playing a similar role if it is present at the C-terminal of dipeptides; therefore we have launched a study of dipeptides of the type L-*X*-L-Pro and the structure of L-Phe-L-Pro has already been reported (Panneerselvam & Chacko, 1989). Here we present the crystal structure of benzyloxycarbonyl-L-alanyl-L-proline (Z-LALP).

Experimental. The dipeptide (Z-LALP) was crystallized in water at room temperature. Colourless chunky crystals, dimensions $0{\cdot}3 \times 0{\cdot}2 \times 0{\cdot}2$ mm. Density measured by the flotation method in carbon tetrachloride and benzene. Three-dimensional intensity data were collected on a Nonius CAD-4 diffractometer. The cell constants were determined by least-squares fit of 20 reflections with 2θ range 20–40°, max. $2\theta = 55°$, ω–2θ scan, data collected for the range $0 \le h \le 11$, $0 \le k \le 28$ and $0 \le l \le 11$. Three standard reflections, 3% variation in intensity. A total of 2213 observations were reduced (Lp^{-1}) to a set of 1511 unique reflections with $I > 3\sigma(I)$ used in the structure determination. The structure was solved using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refinement carried out by full-matrix least-squares method using *SHELX*76 (Sheldrick, 1976).

During the initial isotropic refinement, the C^γ atom of the prolyl residue showed a large temperature factor and the bond lengths involving C^γ had abnormal values. The above features indicated a disorder in the position of the C^γ atom. A difference Fourier map, computed after excluding the C^γ atom from the structure-factor calculation, revealed an

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