conformation is obtained for the O(3)–C(9)–C(10)–C(11) and O(6)–C(24)–C(25)–C(26) angles which avoids steric hindrance of the O atom and the phenyl group. A similar effect is observed in a related compound in the following paper (Bats & Canenbley, 1984).

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[4-(Phenoxymethyl)phenyl]acetic Acid, $C_{15}H_{14}O_3$

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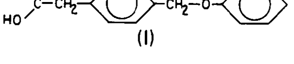
Abstract. $M_r = 242·28$, monoclinic, $P2_1/a$, $a = 6·901$ (1), $b = 6·812$ (3), $c = 26·523$ (4) Å, $\beta = 92·58$ (2)°, $V = 1245·6$ (6) Å^3, $Z = 4$, $D_x = 1·292$ (1) g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0·71069$ Å, $\mu = 0·8$ cm^{-1}, $F(000) = 512$, $T = 293$ K. Final $R = 0·047$ for 1385 independent observed reflections. The molecules form centrosymmetric dimers by hydrogen bonding between two neighboring carboxyl groups. The (phenoxymethyl)phenyl group has the Z conformation required to avoid steric hindrance by the phenyl groups. The dihedral angle between the phenyl groups is 71·1 (2)°, of the same magnitude as the value found in the (benzyloxy)phenyl isomer.

Introduction. The title compound (I) was prepared in view of a possible analgetic activity. Although the compound is closely related to its active isomer [4-(benzyloxy)phenyl]acetic acid (Bats & Canenbley, 1984), no antiphlogistic activity was found. A crystal-structure determination was undertaken to allow for a structural comparison with related compounds.



(I)

Experimental. Synthesis by Canenbley (1983), colorless transparent plates by recrystallization from toluene/ether, crystal used: 0·05 × 0·575 × 0·875 mm, cell constants from setting angles of 25 reflections with $4 < \theta \leq 12°$, CAD-4 diffractometer, graphite monochromator, hemisphere up to $2\theta = 44°$, $(\sin\theta/\lambda)_{\max} = 0·53$ Å^{-1}, range of hkl: h 0→7, k 0→7, l ±27, ω-scan, total number of reflections 3394, independent reflections 1514; three standard reflections every 4500 seconds remained stable; no absorption correction, averaging of equivalent reflections, $R_{\text{int}} = 0·030$, 1385 reflections with $I > 0·3\sigma(I)$ used, weighting scheme $w(I) = 1/[\sigma^2(I) + (0·03I)^2]$, structure determination by *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), all H-atom positions from difference synthesis and included in refinement but their isotropic thermal parameters fixed, refinement on F, extinction coefficient included, $(\Delta/\sigma)_{\max} = 0·2$, final difference Fourier map peaks $<0·15$ e Å^{-3}, final $R = 0·047$, $wR = 0·042$, $S = 1·54$, scattering factors from *International Tables for X-ray Crystallography* (1974), calculations with *SDP* program system (Enraf–Nonius, 1982).

Discussion. The positional parameters are reported in Table 1,* the bond lengths and angles in Table 2. Fig. 1 shows the molecular geometry and numbering scheme.

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* Lists of structure factors, H-atom coordinates and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39237 (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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Table 1. *Positional parameters and equivalent values of the anisotropic thermal parameters*

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

	x	y	z	B_{eq}(Å^2)
O(1)	−0·0344 (2)	−0·0289 (2)	0·56023 (5)	5·18 (4)
O(2)	−0·2519 (2)	0·0688 (3)	0·50205 (5)	5·88 (4)
O(3)	0·0320 (2)	0·0019 (2)	0·80658 (4)	4·15 (3)
C(1)	−0·1986 (3)	0·0187 (3)	0·54827 (7)	4·10 (5)
C(2)	−0·3609 (3)	0·0272 (4)	0·58349 (7)	5·03 (6)
C(3)	−0·3034 (3)	−0·0027 (3)	0·63808 (7)	4·03 (5)
C(4)	−0·3163 (3)	0·1468 (3)	0·67255 (7)	4·82 (6)
C(5)	−0·2655 (4)	0·1169 (4)	0·72292 (7)	4·97 (6)
C(6)	−0·1998 (3)	−0·0623 (3)	0·73998 (7)	3·81 (5)
C(7)	−0·1890 (3)	−0·2120 (3)	0·70560 (7)	4·23 (5)
C(8)	−0·2414 (3)	−0·1830 (3)	0·65554 (7)	4·32 (5)
C(9)	−0·1475 (3)	−0·0964 (4)	0·79444 (7)	4·51 (5)
C(10)	0·1011 (3)	−0·0039 (3)	0·85589 (6)	3·31 (4)
C(11)	0·2711 (3)	0·0958 (3)	0·86639 (7)	3·97 (5)
C(12)	0·3502 (3)	0·1017 (3)	0·91513 (7)	4·39 (5)
C(13)	0·2597 (3)	0·0060 (3)	0·95319 (7)	4·20 (5)
C(14)	0·0930 (3)	−0·0954 (3)	0·94242 (7)	4·06 (5)
C(15)	0·0113 (3)	−0·1024 (3)	0·89381 (6)	3·62 (5)

Table 2. *Bond distances* (Å), *angles and relevant torsion angles* (°)

E.s.d.'s in torsion angles ≃ 0·3°.

C(1)–O(1)	1·207 (2)	C(3)–C(8)	1·374 (3)
C(1)–O(2)	1·309 (2)	C(6)–C(9)	1·491 (2)
O(2)–H(O)	1·02 (2)	C(9)–O(3)	1·432 (2)
C(1)–C(2)	1·491 (3)	O(3)–C(10)	1·373 (2)
C(2)–C(3)	1·498 (2)	C(10)–C(11)	1·373 (2)
C(3)–C(4)	1·374 (3)	C(11)–C(12)	1·381 (2)
C(4)–C(5)	1·381 (2)	C(12)–C(13)	1·375 (3)
C(5)–C(6)	1·372 (3)	C(13)–C(14)	1·361 (3)
C(6)–C(7)	1·372 (2)	C(14)–C(15)	1·385 (2)
C(7)–C(8)	1·375 (2)	C(10)–C(15)	1·378 (2)
C(1)–O(2)–H(O)	108 (1)	C(6)–C(7)–C(8)	121·0 (2)
O(1)–C(1)–O(2)	122·5 (2)	C(7)–C(8)–C(3)	121·2 (2)
O(1)–C(1)–C(2)	124·6 (2)	C(6)–C(9)–O(3)	108·3 (2)
O(2)–C(1)–C(2)	112·9 (2)	C(9)–O(3)–C(10)	117·5 (1)
C(1)–C(2)–C(3)	115·2 (2)	O(3)–C(10)–C(11)	115·9 (2)
C(2)–C(3)–C(4)	121·3 (2)	O(3)–C(10)–C(15)	124·1 (2)
C(2)–C(3)–C(8)	120·8 (2)	C(11)–C(10)–C(15)	120·0 (2)
C(4)–C(3)–C(8)	117·8 (2)	C(10)–C(11)–C(12)	120·2 (2)
C(3)–C(4)–C(5)	120·8 (2)	C(11)–C(12)–C(13)	120·0 (2)
C(4)–C(5)–C(6)	121·1 (2)	C(12)–C(13)–C(14)	119·6 (2)
C(5)–C(6)–C(7)	118·0 (2)	C(13)–C(14)–C(15)	121·2 (2)
C(5)–C(6)–C(9)	121·3 (2)	C(14)–C(15)–C(10)	119·0 (2)
C(7)–C(6)–C(9)	120·7 (2)		
O(1)–C(1)–C(2)–C(3)	7·7	C(7)–C(6)–C(9)–O(3)	108·9
O(2)–C(1)–C(2)–C(3)	−172·3	C(6)–C(9)–O(3)–C(10)	177·0
C(1)–C(2)–C(3)–C(4)	112·6	C(9)–O(3)–C(10)–C(11)	−178·5
C(1)–C(2)–C(3)–C(8)	−69·4	C(9)–O(3)–C(10)–C(15)	1·8
C(5)–C(6)–C(9)–O(3)	−73·1		

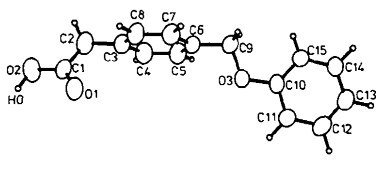

Fig. 1. Perspective view of the molecule and numbering scheme of the atoms.

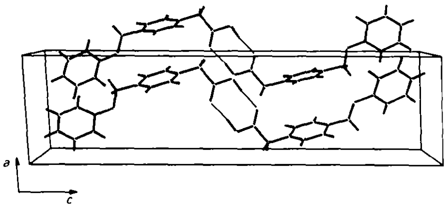

Fig. 2. View of the structure along **b**.

The molecules crystallize as centrosymmetric dimers extended in the crystallographic **c** direction (Fig. 2). The dimerization is achieved by hydrogen bonding between two neighboring carboxyl groups. The characteristic values of the hydrogen bonds are O(2)–H(O): 1·02 (2), O(1)···H(O): 1·63 (2), O(1)···O(2): 2·645 (2) Å, ∠O(2)–H(O)–O(1): 173 (2)°. Thus these bonds are of intermediate strength. The packing among the dimers shows no contacts shorter than the sum of the van der Waals radii of the involved atoms and is thus weak. The relevant torsion angles describing the molecular conformation are given in Table 2. The molecule contains three planar parts: (I) the carboxyl group, (II) phenyl group C(3)–C(8) and (III) phenyl group C(10)–C(15). The dihedral angles between the planes are: (I)/(II) 114·9 (2) and (II)/(III) 71·1 (2)°. The angle (I)/(II) is rather similar to values in the two independent molecules of an isomer (Bats & Canenbley, 1984) although the torsion angles about C(1)–C(2) and C(2)–C(3) are different in all compounds. A perpendicular arrangement was observed in a phenylacetic acid group by Gupta & Sahu (1971). Thus the conformation angles in phenylacetic acid dimers appear rather flexible and considerably affected by crystal-packing forces.

The O(3)–C(9) bond is approximately coplanar with the C(10)–C(15) phenyl group, due to partial double bonding in the C(10)–O(3) bond. The C(10)–O(3)–C(9)–C(6) group has a *Z* conformation which is a requirement to avoid steric hindrance by the phenyl groups. The dihedral angle of 71·1 (2)° between the phenyl groups is of the same magnitude as the value of 64·0 (3)° found in the (benzyloxy)phenyl compound. Although coplanarity of the π-systems is possible in phenoxyacetic acid derivatives (Smith, Kennard & White, 1978), a repulsion between H(7) and O(3) prevents this conformation in the (benzyloxy)phenyl group.

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Polymorphisme du Dihydro-5,6 Pyrimidino[5,4-*c*]carbazole, $C_{14}H_{11}N_3$. I. Structure de la Forme Monoclinique I

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Abstract. $M_r = 221{\cdot}3$, $P2_1/c$, $a = 9{\cdot}127\,(4)$, $b = 9{\cdot}390\,(4)$, $c = 14{\cdot}903\,(8)$ Å, $\beta = 119{\cdot}30\,(4)°$, $V = 1114\,(2)$ Å^3, $Z = 4$, $D_m = 1{\cdot}28\,(2)$, $D_x = 1{\cdot}31$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}088$ mm^{-1}, $F(000) = 464$, 294 K, final $R = 0{\cdot}055$ for 1474 independent reflections. The structure consists of chains of molecules linked by N—H···N hydrogen bonds of 2·867 (4) Å. The pyrimidine, pyrrole and benzene rings are planar and have normal bond lengths and angles. The cyclohexadiene ring has a half-chair conformation as is found in 1,3-cyclohexadiene although the bond lengths are different.

Introduction. La synthèse d'hétérocycles nouveaux susceptibles d'intercalation dans l'acide désoxyribonucléïque et à visée oncostatique nous a conduit à l'étude de structures tétracycliques inspirées du modèle de l'ellipticine et édifiées par l'adjonction de la pyrimidine au carbazole (Robba & Boutamine, 1976).

Les premiers résultats observés dans le cas de quelques dérivés au cours des essais sur la leucémie lymphocytaire P 388 de la souris, nous ont orientés vers l'étude radiocristallographique du dihydro-5,6 pyrimidino[5,4-*c*]carbazole en vue de déterminer la relation entre la conformation moléculaire et l'activité pharmacologique au niveau du site récepteur, d'autant que ce composé se présente sous différentes variétés polymorphiques (Nguyen-Huy Dung & Lancelot, 1984). Toutes ces considérations nous ont amenés à étudier par diffraction de RX la structure cristalline sur un monocristal de l'hétérocycle obtenu par recristallisation dans l'acétone.

Partie expérimentale. Mesure de la masse volumique par flottation; dimensions du cristal: 150 × 250 × 300 µm; dimensions de la maille déterminées sur monocristal à partir de 15 réflexions avec le rayonnement Mo $K\alpha$ ($5{,}4 \leq \theta \leq 14{,}0°$); diffractomètre automatique CAD-4 Enraf–Nonius, balayage θ–2θ d'amplitude $s(°) = 2{,}30 + 0{,}75\mathrm{tg}\theta$; $0 \leq 2\theta \leq 56°$; $-12 \leq h \leq +12$; $0 \leq k \leq 12$; $0 \leq l \leq 19$; pas de corrections d'absorption; réflexions choisies pour contrôler les intensitiés: $31\bar{8}$, $\bar{4}18$, $41\bar{6}$, écart-type relatif moyen sur les intensités de ces réflexions 0,04; nombre de réflexions indépendantes mesurées: 2674; nombre de réflexions considérées comme observées $[I > 2\sigma(I)]$: 1474; résolution de la structure: méthode directe à l'aide de *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); affinement basé sur F par la méthode des moindres carrés à l'aide du programme à matrice complète de Busing (1971); les coordonnées des atomes d'azote et

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