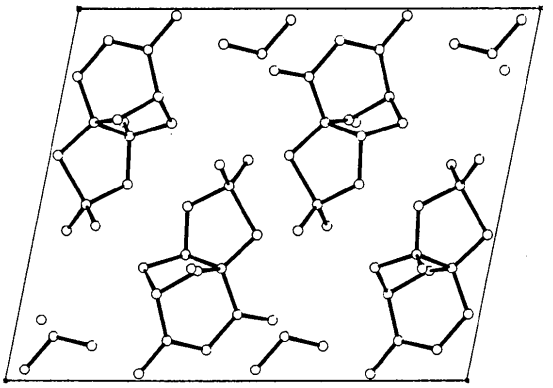

Fig. 2. *b*-axial projection of the unit-cell contents.

The structure determination confirms the molecular structure shown for (5) and provides the first example of a saturated cyclic sultone, although there are two examples where partly unsaturated sultone rings have been reported (Barnett, Newton & McCormack, 1972; Beetz, Kellogg, Kiers & Piepenbroek, 1975). The mean acyclic S—O bond is 1·417 (4) Å which compares with values of 1·43 and 1·41 Å quoted by Beetz *et al.* The cyclic S—O bond length of 1·559 (3) Å is slightly shorter than the values found by Barnett *et al.* and by Beetz *et al.*, 1·577 and 1·59 Å, respectively. The S—C bond length of 1·772 (7) Å compares with that of 1·727 Å reported by Barnett *et al.* There were no abnormal intermolecular contact distances.

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4-Hydroxy-4-phenylpentanamide, $C_{11}H_{15}NO_2$, a Moderately Active Anticonvulsant

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Abstract. $M_r = 193{\cdot}25$, monoclinic, $P2_1/n$, $a = 24{\cdot}215$ (4), $b = 6{\cdot}981$ (2), $c = 6{\cdot}147$ (1) Å, $\beta = 91{\cdot}7$ (1)°, $V = 1038{\cdot}7$ (6) Å^3, $Z = 4$, $D_m = 1{\cdot}23$, $D_x = 1{\cdot}24$ Mg m^{-3}, graphite-monochromatized Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 0{\cdot}61$ mm^{-1}, $F(000) = 416$, $T = 296$ K, $R = 0{\cdot}058$, $R_w = 0{\cdot}053$ for 1091 observed reflections ($I > 3\sigma$) and 187 refined parameters. The molecule adopts a pseudocyclic conformation through hydroxyl···amide oxygen intramolecular hydrogen bonding. The distance of 6·10 (1) Å between the centroid of the phenyl ring and the electron-donating oxygen atom is in the range found for other anticonvulsants.

Introduction. The title compound [also known as γ-hydroxy-γ-methyl-γ-phenylbutyramide (HMPB)] has long been known for its anticonvulsant activity. It produces a reduction in the duration of convulsions on

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

	x	y	z	B_{eq}(Å^2)*
C(1)	890 (2)	−338 (8)	2482 (8)	4·7 (2)
C(2)	1062 (1)	920 (5)	578 (5)	3·1 (1)
C(3)	861 (2)	2985 (6)	969 (7)	3·8 (1)
C(4)	1023 (2)	4460 (6)	−733 (8)	4·2 (2)
C(5)	615 (2)	4668 (6)	−2569 (6)	3·5 (1)
C(6)	1687 (1)	880 (4)	366 (5)	2·8 (1)
C(7)	1929 (2)	195 (5)	−1504 (6)	3·5 (1)
C(8)	2498 (2)	205 (6)	−1681 (7)	4·2 (2)
C(9)	2833 (2)	902 (6)	−39 (7)	4·4 (2)
C(10)	2596 (2)	1573 (6)	1852 (7)	4·3 (2)
C(11)	2034 (2)	1546 (5)	2025 (7)	3·6 (1)
O(1)	799 (1)	147 (4)	−1341 (4)	3·7 (1)
O(2)	381 (1)	3241 (3)	−3390 (4)	5·1 (1)
N(1)	515 (2)	6424 (5)	−3335 (6)	3·9 (1)

* $B_{eq} = \frac{4}{3}\sum_{ij} T_{ij} B_{ij}$.

Table 2. *Relevant bond angles* (°) *with e.s.d.'s in parentheses*

C(1)–C(2)–C(3)	108·8 (3)	C(3)–C(4)–C(5)	114·1 (4)
C(1)–C(2)–C(6)	110·4 (3)	C(4)–C(5)–O(2)	120·9 (3)
C(1)–C(2)–O(1)	106·8 (3)	C(4)–C(5)–N(1)	117·9 (4)
C(3)–C(2)–C(6)	110·4 (3)	O(2)–C(5)–N(1)	121·1 (3)
C(3)–C(2)–O(1)	110·3 (3)	C(2)–C(6)–C(7)	121·4 (3)
C(6)–C(2)–O(1)	110·0 (3)	C(2)–C(6)–C(11)	121·0 (3)
C(2)–C(3)–C(4)	115·8 (3)		

both tonic and clonic phases elicited by electroshock, which is considered an experimental model of the *grand-mal* epilepsy. The compound, however, shows no protection against the convulsions induced by thiosemicarbazide and pentylenetetrazole (Carvajal, Russek, Tapia & Massieu, 1964). It was previously named MPP because it was believed to be 5-methyl-5-phenyl-2-pyrrolidinone, a cyclic analogue of γ-aminobutyric acid, when it was designed and synthesized to penetrate the blood–brain barrier to inhibit γ-aminobutyric acid transaminase. Its structure has only recently been revised by proton and carbon magnetic resonance (Joseph-Nathan, Massieu & Carvajal, 1978) to establish its structural formula as HMPB. The geometrical configuration of this substance may be of aid to the understanding of its mechanism of action at a molecular level. For this reason and to confirm its structural formula unambiguously its crystal structure determination was undertaken.

Experimental. D_m by flotation, prismatic colourless crystals, 0·20 × 0·20 × 0·30 mm, Nonius CAD-4 diffractometer, cell parameters by least squares on setting angles for 25 reflections $20 < 2\theta < 50°$, intensities by ω–2θ scans for $\omega = (0{\cdot}80 + 0{\cdot}14\tan\theta)°$ at ω speed of 6·7° min^{-1} max.; 3 standard reflections varied ±2% of mean intensities; hkl and $hk\bar{l}$ to $\theta = 55°$, 1307 independent reflections, 1092 observed above $3\sigma(I)$ level, Lp correction but not absorption; structure solved by direct methods, H atoms located in a difference map; anisotropic least-squares refinement (isotropic for H) minimizing $\sum w(|F_o| - |F_c|)^2$, $w = 1/\sigma^2(F_o)$, excluding unobserved and one strong reflection (600); $R = 0{\cdot}058$ for observed reflections, $R_w = 0{\cdot}053$, max. $\Delta/\sigma = 0{\cdot}002$, $\Delta\rho$ excursions within −0·23 and 0·19 e Å^{-3}, scattering factors for C, N and O from Cromer & Mann (1968) with corrections for anomalous dispersion from Cromer & Liberman (1970), for H from Stewart, Davidson & Simpson (1965); *SHELX* (Sheldrick, 1976) system of programs and *ORTEP* (Johnson, 1965).*

Discussion. The final atomic parameters for non-H atoms are given in Table 1, and a projection of the molecular structure is shown in Fig. 1 together with atomic numbering and bond distances. Relevant angles

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39085 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

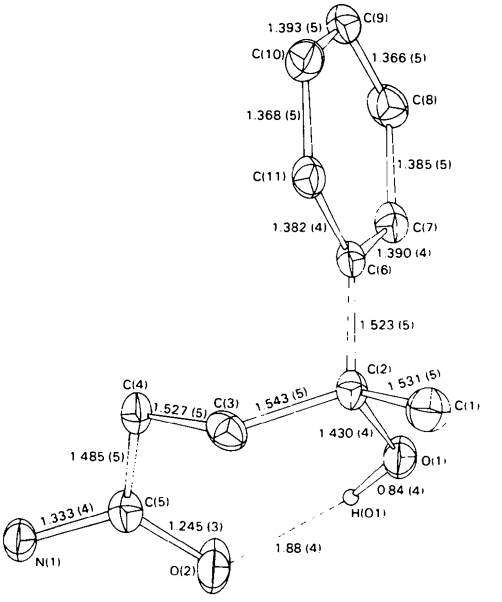

Fig. 1. Projection of the molecular structure, with the thermal ellipsoids drawn at 45% probability, except H(O1), showing bond distances (Å) with e.s.d.'s in parentheses.

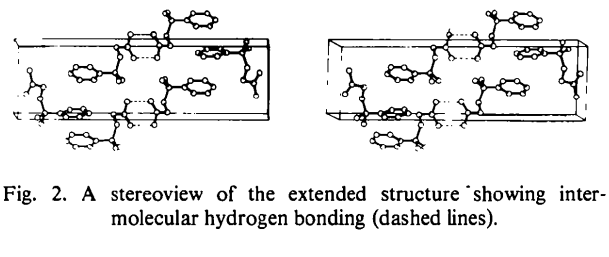

Fig. 2. A stereoview of the extended structure showing intermolecular hydrogen bonding (dashed lines).

between non-H atoms are given in Table 2. The phenyl ring is planar to within experimental accuracy. The amide group is also planar, with deviations from the best least-squares plane of N(1) +0·018 (4), C(5) −0·014 (4), H(N1) −0·01 (4), H′(N1) −0·00 (4), O(2) +0·007 (3) Å. The amide moiety folds back and forms a 'seven-atom ring' with the open end closed by an intramolecular hydrogen bond [O(1)···O(2) = 2·683 (4), H(O1)–O(1) = 0·84 (4), H(O1)···O(2) = 1·88 (4) Å, O(1)–H(O1)···O(2) = 160 (4)°]. The C(5)–O(2) acceptor bond of 1·245 (3) Å and the C(2)–O(1) donor bond of 1·430 (4) Å are in good agreement, to within experimental accuracy, with the expected bond lengths caused by hydrogen-bond formation (Jeffrey, Ruble, McMullan, DeFrees, Binkley & Pople, 1980).

A stereopicture of the extended structure is shown in Fig. 2. The dihedral angle between phenyl rings of neighbouring molecules is 47 (1)°. The carbon chains in the unit cell lie approximately along **c**. This arrangement favours a weak intermolecular hydrogen bonding between molecules of neighbouring unit cells [N(1)···O(2) = 2·925 (5), H(N1)–N(1) = 1·02 (4), H(N1)···O(2) = 1·91 (4) Å, N(1)–H(N1)···O(2) = 174 (3)°].

The distance between the centroid of the aromatic ring and the electron-donor oxygen [O(2)], believed to be of significance in the biological activity of the molecule, is 6·10 (1) Å, a value in the range found for phenacemide (6·39 Å) and ethylphenacemide (5·85 Å), two potent anticonvulsant agents (Camerman & Camerman, 1977).

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The Structures of 3-Allyl-9-benzoyl-2-methyl-9-phenyl-4,9-dihydropyrazolo[5,1-*b*]-quinazoline, $C_{27}H_{23}N_3O$, and 6,7-Dimethyl-1,3,3-triphenyl-1*H*-imidazo[1,2-*b*]pyrazol-2(3*H*)-one, $C_{25}H_{21}N_3O$

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Abstract. $C_{27}H_{23}N_3O$ (2*b*): $M_r = 405·5$, orthorhombic, *Pbca*, $a = 13·025$ (4), $b = 15·991$ (3), $c = 20·593$ (6) Å at 297 K, $V = 4289$ (2) Å^3, $Z = 8$, $D_x = 1·26$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0·64$ cm^{-1}, $F(000) = 1712$; R_F for 1671 unique reflections $[I \geq 2\sigma(I)] = 0·0728$. $C_{25}H_{21}N_3O$ (3*a*), $M_r = 379·5$, monoclinic, $P2_1/c$, $a = 11·234$ (4), $b = 7·021$ (1), $c = 25·330$ (6) Å, $\beta = 91·83$ (3)° at 299 K, $V = 1997$ (1) Å^3, $Z = 4$, $D_x = 1·26$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0·70$ cm^{-1}, $F(000) = 800$; R_F for 1383 unique reflections $[I \geq 2·75\sigma(I)] = 0·0770$. Bond distances and angles are all within the expected ranges. The 1,2-diazacyclopentadiene rings in both structures are nearly planar.

Introduction. The antineoplastic activity of the imidazo[1,2-*b*]pyrazole ring system has received considerable attention during the past few years (Shoemaker, Ayers, D'Anna & Cysyk, 1981; Cory & Fleischer, 1980; Allen & Thornthwaite, 1980). The known medicinal activity of fused pyrazoles has spurred considerable research into the synthesis of imidazo[1,2-*b*]pyrazoles (Elnagdi, Hafez & El-Fahham, 1980; Pilgram, 1980; Elguero, Jacquier & Mignonac-Mondon, 1973; Schulze & Willitzer, 1967) as well as the pyrazolo[5,1-*b*]-quinazolines (Sircar, Capiris, Kesten & Herzig, 1981; Puetter, Wolfrum & Menzee, 1963) which appear in this paper. It has been suggested that the antitumor

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