

176 (3)^o]. In the crystal packing, intermolecular hydrogen bonds are also formed for the atomic pairs N(14)⋯O(21) and N(16')⋯O(20'): N(14)(*x*, *y*, *z*)⋯O(21)(*x*, *y*, *z* - 1) = 2.623 (6) and N(16')(*x*, *y*, *z*)⋯O(20')(*x*, *y*, *z* - 1) = 2.546 (6) Å.

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Structure of a Cyclic Kynurenine Derivative

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Abstract. (2-Oxo-2,3,4,5-tetrahydro-1*H*-1-benzazepin-1-yl)ethanoic acid, C₁₂H₁₃NO₃, *M_r* = 219.2, orthorhombic, *Pbca*, *a* = 15.230 (1), *b* = 10.196 (1), *c* = 28.267 (2) Å, *U* = 4389.4 (1) Å³, *D_m* (floatation) = 1.32 (1), *D_x* = 1.327 Mg m⁻³, *Z* = 16, λ(Cu *Kα*) = 1.5418 Å, μ = 0.70 mm⁻¹, *F*(000) = 1856, *T* = 294 (1) K, final *R* = 0.061 for 2772 observed data. The two independent molecules adopt essentially similar conformations. The seven-membered heterocyclic rings are in a boat form, and the aromatic rings are planar within the limits of experimental error. The carboxylate group of one of the molecules assumes two orientations in the crystal with occupancies of 0.34 (1) and 0.66 (1).

Introduction. As part of a program in which we are defining conformational detail for a number of cyclic derivatives of kynurenine (I), a major metabolic and oxidative degradation product of the amino acid tryptophan, we report here the structure of (2-oxo-2,3,4,5-tetrahydro-1*H*-1-benzazepin-1-yl)ethanoic acid (II). Because of the structural similarities of these kynurenine derivatives to the

biologically active seven-membered nitrogen heterocycles, they are of considerable pharmacological interest. Their relationship to the biologically active 1,4-benzodiazepines, which exhibit anxiolytic effects on the central nervous system (Hoffmeister & Stille, 1981), has rendered the cyclic kynurenines of particular interest as potential sources of *natural* anxiolytic agents.

Experimental. (II) was synthesized by standard base-catalysed hydrolysis of benzyl (2-oxo-2,3,4,5-tetrahydro-1*H*-1-benzazepin-1-yl)ethanoate obtained from 2-oxo-2,3,4,5-tetrahydro-1*H*-1-benzazepine (Tomita, Minami & Uyeo, 1969). A colourless triangular platelet of side *ca* 0.63 mm and 0.13 mm thick, crystallized from aqueous ethanol, was aligned on a Rigaku-AFC diffractometer; cell parameters determined by least squares from 2θ values for 25 strong reflections (35° < 2θ < 75°); Cu *Kα* radiation (graphite crystal monochromator, λ = 1.5418 Å); ω-2θ scan, scan rate 4° min⁻¹, scan range (Δω) (1.2 + 0.5 tan θ)°, 2θ_{max} = 130°, 10 s stationary background counts; three standard reflections monitored

every 50 reflections, no significant intensity variation; 4133 unique data, h 0 to 17, k 0 to 33, l 0 to 12, 2722 for which $I > \sigma I$ used for refinement; intensities corrected for Lorentz and polarization effects and for absorption, transmission factors 0.767 to 0.921. Structure solved by direct methods with *SHELXS86* (Sheldrick, 1985) and refined with *SHELX76* (Sheldrick, 1976). During refinement, the high thermal parameters of the carboxyl group of atoms of molecule *A* and the residual electron density in the difference map indicated disorder in which the carboxyl group assumes two alternate orientations in the crystal. The structural model was therefore adjusted to include two sites for these atoms with occupancies which refined to values of 0.34 (1) and 0.66 (1); the coordinates of these atoms were not refined. H atoms, apart from those of the disordered carboxylic acid group, were located on difference maps and their parameters refined. Refinement with anisotropic temperature factors given to all C, O and N atoms converged at $R = 0.061$, $wR = 0.076$, $S = 1.40$ (401 parameters varied); function minimized $\sum w(|\Delta F|)^2$ with $w = [\sigma^2(|F|) + 0.0014|F|^2]^{-1}$; $(\Delta\rho)_{\max}$, $(\Delta\rho)_{\min} = +0.36, -0.36 \text{ e } \text{\AA}^{-3}$; $(\Delta/\sigma)_{\max} = 0.04$; an isotropic extinction correction of the form $F = F_c[1 - (4.95 \times 10^{-7} F^2/\sin\theta)]$ was applied to the calculated structure amplitudes. Atomic scattering factors and anomalous-dispersion factors from *International Tables for X-ray Crystallography* (1974). Figures were prepared from the output of *ORTEPII* (Johnson, 1976). Calculations performed on a VAX11/780 computer.

Discussion. Final atomic coordinates for the non-H atoms are given in Table 1.* The molecular conformation and numbering scheme are illustrated in Fig. 1, while bond lengths, valence angles and selected torsion angles are given in Table 2.

The two independent molecules (*A* and *B*) adopt a similar conformation with the seven-membered heterocyclic ring in a boat form. The bow and stern angles of the boat, in this case the angles between the mean central plane comprising atoms N(1), C(2), C(4), C(5) and the planar atom groupings C(2), C(3), C(4) and N(1), C(9*a*), C(5*a*), C(5) respectively, have values of 49.6 (8) and 52.8 (8)° for molecule *A* and 48.6 (8) and 52.2 (8)° for molecule *B*. The values for the bow angles are less than those for several 2,5-dioxo-2,3,4,5-tetrahydro-1*H*-1-benzazepines whose values range from 59.7 (5) to 63.8 (6)° (see Table 3),

* Lists of structure amplitudes, anisotropic thermal parameters, H-atom coordinates and short intermolecular approaches have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52944 (32 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

Atoms of molecule *A* are numbered 1 to 13 and those of molecule *B* 21 to 33. $B_{\text{eq}} = (8\pi^2/3)\sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$.

	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}}(\text{\AA}^2)$
N(1)	-2346 (2)	-4089 (2)	6070 (1)	3.37 (4)
C(2)	-1602 (2)	-3395 (3)	6130 (1)	4.01 (6)
O(2)	-1243 (2)	-3376 (2)	6524 (1)	5.53 (5)
C(3)	-1234 (3)	-2692 (4)	5710 (2)	5.04 (8)
C(4)	-796 (3)	-3625 (5)	5357 (2)	6.34 (10)
C(5)	-1362 (2)	-4843 (4)	5254 (2)	5.71 (9)
C(5 <i>a</i>)	-2324 (2)	-4526 (3)	5220 (1)	4.24 (6)
C(6)	-2793 (3)	-4573 (4)	4794 (1)	5.68 (9)
C(7)	-3680 (3)	-4286 (4)	4773 (2)	5.95 (9)
C(8)	-4117 (3)	-3965 (4)	5179 (1)	5.20 (8)
C(9)	-3680 (2)	-3898 (3)	5599 (1)	4.06 (6)
C(9 <i>a</i>)	-2789 (2)	-4172 (3)	5620 (1)	3.40 (5)
C(10)	-2696 (3)	-4776 (4)	6480 (1)	4.20 (6)
C(11)*	-2236 (0)	-5689 (0)	6739 (0)	4.81 (24)
C(11)†	-1970 (0)	-5806 (0)	6573 (0)	7.55 (20)
O(12)*	-1684 (0)	-6300 (0)	6498 (0)	3.41 (13)
O(12)†	-1625 (0)	-6460 (0)	6247 (0)	5.61 (9)
O(13)*	-2388 (0)	-6055 (0)	7161 (0)	4.89 (14)
O(13)†	-1913 (0)	-6260 (0)	6996 (0)	6.25 (10)
N(21)	-822 (2)	-1377 (2)	3055 (1)	3.55 (5)
C(22)	-193 (2)	-2285 (3)	3136 (1)	4.01 (6)
O(22)	582 (1)	-2023 (2)	3034 (1)	5.53 (5)
C(23)	-480 (3)	-3574 (3)	3341 (1)	4.65 (7)
C(24)	-668 (3)	-3477 (4)	3876 (1)	5.23 (8)
C(25)	-1173 (3)	-2231 (4)	4005 (1)	4.65 (7)
C(25 <i>a</i>)	-1904 (2)	-1937 (3)	3664 (1)	3.79 (6)
C(26)	-2778 (3)	-2080 (4)	3793 (2)	5.11 (8)
C(27)	-3452 (3)	-1861 (4)	3472 (2)	5.96 (9)
C(28)	-3252 (3)	-1502 (4)	3021 (2)	5.89 (9)
C(29)	-2386 (2)	-1350 (4)	2882 (1)	4.88 (7)
C(29 <i>a</i>)	-1714 (2)	-1566 (3)	3203 (1)	3.67 (6)
C(30)	-556 (2)	-131 (3)	2843 (1)	3.92 (6)
C(31)	-39 (2)	707 (3)	3186 (1)	3.61 (6)
O(32)	-11 (2)	553 (2)	3605 (1)	4.77 (5)
O(33)	361 (2)	1670 (3)	2955 (1)	5.19 (5)

* Atom included with occupancy factor 0.34 (1).

† Atom included with occupancy factor 0.66 (1).

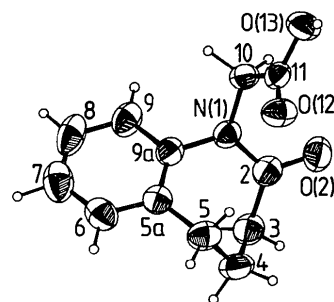


Fig. 1. Perspective view of molecule *B* with thermal ellipsoids scaled to 50% probability. The C symbol is omitted and H atoms are denoted by spheres of arbitrary radius.

whilst the stern angles are considerably larger [*cf.* values 18.2 (5) to 27.1 (6)°]. In 3-chloro-*N*-(2,5-dioxo-2,3,4,5-tetrahydro-1*H*-1-benzazepin-3-yl)benzamide (Gulbis, Mackay & Rivett, 1990) the heterocyclic ring adopts a slightly different conformation which can be described as twist boat. The conformation of the benzazepine ring in (II), however, is very similar to its conformation in 2-oxo-2,3,4,5-tetrahydro-1,5-ethanobenzazepine (Somayaji, Skorey,

Table 2. Bond lengths (Å), valence and selected torsion angles (°) for (II) with *e.s.d.*'s in parentheses

	Molecule A	Molecule B	
N(1)—C(2)	1.347 (4)	1.351 (4)	
N(1)—C(9a)	1.442 (4)	1.434 (4)	
N(1)—C(10)	1.455 (4)	1.462 (4)	
C(2)—O(2)	1.243 (4)	1.244 (3)	
C(2)—C(3)	1.496 (6)	1.501 (4)	
C(3)—C(4)	1.532 (7)	1.542 (4)	
C(4)—C(5)	1.540 (6)	1.530 (6)	
C(5)—C(5a)	1.503 (4)	1.503 (5)	
C(5a)—C(6)	1.401 (4)	1.388 (6)	
C(5a)—C(9a)	1.382 (4)	1.387 (4)	
C(6)—C(7)	1.385 (6)	1.388 (7)	
C(7)—C(8)	1.366 (6)	1.361 (8)	
C(8)—C(9)	1.363 (4)	1.386 (6)	
C(9)—C(9a)	1.387 (4)	1.387 (4)	
C(10)—C(11)*	1.38, 1.55	1.511 (4)	
C(11)—O(12)*	1.25, 1.25	1.196 (4)	
C(11)—O(13)*	1.27, 1.28	1.327 (4)	
C(2)—N(1)—C(9a)	122.4 (2)	122.1 (1)	
C(2)—N(1)—C(10)	117.4 (2)	117.9 (2)	
C(9a)—N(1)—C(10)	120.2 (2)	119.9 (2)	
N(1)—C(2)—O(2)	119.4 (2)	119.1 (2)	
N(1)—C(2)—C(3)	117.8 (3)	117.3 (2)	
O(2)—C(2)—C(3)	122.7 (3)	123.6 (2)	
C(2)—C(3)—C(4)	112.5 (3)	112.1 (3)	
C(3)—C(4)—C(5)	112.4 (4)	112.3 (3)	
C(4)—C(5)—C(5a)	112.6 (3)	112.7 (3)	
C(5)—C(5a)—C(6)	123.0 (3)	121.4 (3)	
C(5)—C(5a)—C(9a)	120.2 (2)	120.2 (2)	
C(6)—C(5a)—C(9a)	116.8 (2)	118.4 (3)	
C(5a)—C(6)—C(7)	121.8 (3)	121.4 (3)	
C(6)—C(7)—C(8)	119.3 (3)	119.3 (4)	
C(7)—C(8)—C(9)	120.4 (3)	120.7 (3)	
C(8)—C(9)—C(9a)	120.3 (2)	119.8 (3)	
N(1)—C(9a)—C(5a)	119.8 (2)	120.4 (2)	
N(1)—C(9a)—C(9)	118.9 (2)	119.2 (2)	
C(5a)—C(9a)—C(9)	121.3 (2)	120.4 (2)	
N(1)—C(10)—C(11)*	124, 102	111.9 (2)	
C(10)—C(11)—O(12)*	113, 127	125.3 (2)	
C(10)—C(11)—O(13)*	122, 117	110.0 (2)	
O(12)—C(11)—O(13)*	119, 118	124.6 (2)	
N(1)—C(2)—C(3)—C(4)	-74.3 (5)	-77.1 (4)	-71†
C(2)—C(3)—C(4)—C(5)	46.2 (5)	42.5 (4)	49
C(3)—C(4)—C(5)—C(5a)	39.1 (5)	42.9 (4)	43
C(4)—C(5)—C(5a)—C(6)	110.1 (4)	109.0 (4)	105
C(4)—C(5)—C(5a)—C(9a)	-70.1 (5)	-68.3 (4)	-73
C(5)—C(5a)—C(9a)—N(1)	0.9 (5)	-4.1 (4)	-7
C(5a)—C(9a)—N(1)—C(2)	51.4 (4)	50.5 (4)	71
C(9a)—N(1)—C(2)—C(3)	0.0 (5)	6.3 (4)	-12
C(2)—N(1)—C(9a)—C(9)	-128.9 (3)	-130.7 (3)	-112
C(9)—C(9a)—N(1)—C(10)	51.5 (4)	54.0 (4)	
C(10)—N(1)—C(2)—O(2)	0.6 (4)	1.0 (4)	
C(5a)—C(9a)—N(1)—C(10)	-128.2 (3)	-124.9 (3)	
C(9a)—N(1)—C(10)—C(11)*	123, 114	104.3 (3)	
N(1)—C(10)—C(11)—O(12)*	-30, -45	-16.4 (4)	
C(10)—N(1)—C(2)—C(3)	179.6 (3)	-178.3 (3)	
C(2)—N(1)—C(10)—C(11)*	-57, -66	-71.2 (3)	

* Values for the two carboxylate orientations in molecule *A* are included.

† Values for 2-oxo-2,3,4,5-tetrahydro-1,5-ethanobenzazepine (Somayaji, Skorey, Brown & Ball, 1986).

Table 3. Interplanar angles (°) in the seven-membered heterocycles of 2,5-dioxo- and 2-oxo-2,3,4,5-tetrahydro-1*H*-1-benzazepines

Compound	Bow	Stern
(1) 1,1-Dimethylethyl- <i>N</i> -(2,5-dioxo-2,3,4,5-tetrahydro-1 <i>H</i> -1-benzazepin-3-yl)carbamate	60.2 (5) 59.7 (5)	18.2 (5) 27.2 (5)
(2) 2-Amino- <i>N</i> -(2,5-dioxo-2,3,4,5-tetrahydro-1 <i>H</i> -1-benzazepin-3-yl)benzamide	60.6 (10)	26.9 (10)
(3) <i>N</i> -(2,5-Dioxo-2,3,4,5-tetrahydro-1 <i>H</i> -1-benzazepin-3-yl)-2-naphthamide	63.8 (6)	27.1 (6)
(4) 2-Oxo-2,3,4,5-tetrahydro-1,5-ethanobenzazepine	49.9	62.4
(5) (2-Oxo-2,3,4,5-tetrahydro-1 <i>H</i> -1-benzazepin-1-yl)ethanoic acid	49.6 (8) 48.6 (6)	52.8 (8) 52.2 (8)

References: (1) Ball, Wong, Capuano, Gulbis, Mackay & Alewood (1990); (2), (3) Gulbis, Mackay & Rivett (1990); (4) Somayaji, Skorey, Brown & Ball (1986); (5) this work.

aromatic ring atoms (coplanar to within the limits of experimental error) are 51.2 (8) and 53.2 (8)° in molecules *A* and *B* respectively, and the ethanoic acid plane comprising atoms C(10), C(11), O(12) and O(13) [coplanar within ± 0.04 , ± 0.10 Å for molecule *A* and ± 0.01 (1) Å for molecule *B*] is approximately orthogonal to it; the interplanar angles are *ca* 78° (molecule *A*) and 99.7 (7)° (molecule *B*).

The bond lengths and angles (Table 2) are in good agreement with values reported for related structures. A shortening of the C(9a)—N(1) bond length from the normal single-bond value of 1.470 (5) Å, proposed by Camerman (1970), to a mean value of 1.438 (4) Å for the two independent molecules, is indicative of some electron delocalization between the amide group and its associated aromatic ring. This is accompanied by a lengthening of the C(2)—O(2) bond to a mean value of 1.244 (4) Å. Similar features were also noted in the 2,5-dioxo-2,3,4,5-tetrahydro-1*H*-1-benzazepines (Ball, Wong, Capuano, Gulbis, Mackay & Alewood, 1990; Gulbis, Mackay & Rivett, 1990). Relative to the latter, in which the endocyclic angle C(2)—N(1)—C(9a) ranged in value from 128.7 (2) to 134.2 (3)°, this angle in (II), in which the nitrogen is bonded to an ethanoic acid moiety instead of an H atom, has contracted to a mean value of 122.2 (2)°. The trigonal planar arrangement about the ring nitrogen in (II) [torsion angle C(10)—N(1)—C(2)—C(9a) 175° (molecule *A*) and 180° (molecule *B*)] and in the other 2,5-dioxo-2,3,4,5-tetrahydro-1*H*-1-benzazepines contrasts with the approximate tetrahedral arrangement about this nitrogen in the 2-oxo-2,3,4,5-tetrahydro-1,5-ethanobenzazepine structure (Somayaji, Skorey, Brown & Ball, 1986), which no doubt is a consequence of the 1,5-dimethylene bridge across the seven-membered ring.

The crystal packing is illustrated in Fig. 2. Hydrogen bonds link the *A* molecules to *B* molecules

Brown & Ball, 1986) in which the bow and stern angles have the respective values of 50 and 62°, as compared with values reported for a number of 1,4-benzodiazepines which range from 53.4 (7) to 57.5 (7)° (bow) and from 33.0 (12) to 38.8 (12)° (stern) (Hamor & Martin, 1983; Butcher & Hamor, 1984; Kemmish & Hamor, 1988, 1989). The six atoms C(9a), N(1), C(10), C(2), O(2) and C(3) in (II) form a plane with a r.m.s.d. of 0.004 Å (δ_{\max} 0.006 Å) for molecule *A* and a r.m.s.d. of 0.033 Å (δ_{\max} 0.046 Å) for molecule *B*. The angles between the perpendiculars to this plane and that of the

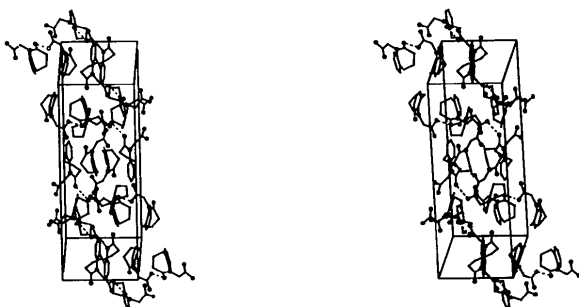


Fig. 2. Stereoview of the crystal packing. Direction of projection a axis, the c axis is vertical. Only one carboxylate orientation is indicated for molecule A .

of the other mirror image conformer to form chains extending along the $[010]$ direction, the chains being held together by van der Waals forces. For the hydrogen-bonding interactions, a carboxylate oxygen is the donor atom to the ring carbonyl oxygen of an adjacent molecule; the $O(12)\cdots O(22)$, $O'(13)\cdots O(22)$ and $O(33)\cdots O(2)$ distances are 2.74, 2.68 and 2.644 (4) Å respectively, with the $O(33)-H(O33)$ and $H(O33)\cdots O(2)$ spacings 0.96 (6) and 1.72 (6) Å and the $O(33)-H(O33)\cdots O(2)$ angle 161 (4)°.

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Structure of 3,6-Diphenylpyrrolo[3,4-*c*]pyrrole-1,4-dithione

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Abstract. The crystal structure of 3,6-diphenylpyrrolo[3,4-*c*]pyrrole-1,4-thione has been determined. There are two different crystal forms, both of which are monoclinic. The crystal data are: $C_{18}H_{12}N_2S_2$, $M_r = 320.426$; modification (I), $P2_1/n$, $a = 7.986$ (1), $b = 4.757$ (1), $c = 19.685$ (3) Å, $\beta = 99.18$ (2)°, $V = 738.2$ (5) Å³, $Z = 2$, $D_x = 1.441$, $D_m = 1.432$ Mg m⁻³, graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $T = 293$ K, $F(000) = 332$, $\mu = 0.342$ mm⁻¹, $R = 0.064$ for 1208 reflexions; modification (II), $P2_1/n$, $a = 4.873$ (1), $b = 18.613$ (2), $c = 7.995$ (1) Å, $\beta = 95.76$ (2)°, $V = 721.5$ (5) Å³, $Z = 2$, $D_x = 1.475$, $D_m = 1.465$ Mg m⁻³, graphite-mono-

chromated Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $T = 293$ K, $F(000) = 332$, $\mu = 0.350$ mm⁻¹, $R = 0.054$ for 877 reflexions. The crystal forms are similar but differ slightly in the following points: both phenyl rings are twisted out of the plane of the heterocyclic ring system by 13° in modification (I), and by only 6° in modification (II). In the projection along the stacking axis, all the molecules are arranged in parallel in modification (I), and in a zigzag arrangement in modification (II).

Introduction. 3,6-Diphenylpyrrolo[3,4-*c*]pyrrole-1,4-dithione (DPPT, Fig. 1) is a thionated derivative of

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