

Crystal packing is stabilized by O—H...O hydrogen bonding (Fig. 2). The water molecule is H bonded with the coumarin molecule of the same asymmetric unit [O(13)...OW = 2.587 (4), O(13)—H = 0.86 Å, O(13)—H...OW = 173.2 (2)°]. In addition, the water molecule is also involved in an intermolecular hydrogen bond with the glide-related coumarin molecule {OW...O(2ⁱ) = 2.773 (4), OW—H(OW) = 0.96 Å, OW—H...O(2ⁱ) = 151.5 (2)° [symmetry code: (i) $-x, \frac{1}{2} + y, -z$]}. Yet another possible H bond is present between the water molecule and the 7-hydroxy group but could not be fully characterized owing to the non-location of the second H atom on the water molecule from the difference maps {the short contact is OW...O(7ⁱⁱ) = 2.890 (4) Å [symmetry code: (ii) $-x + 1, y - \frac{1}{2}, -z$]}. The characteristic O—H...O hydrogen bond observed in 7-hydroxycoumarins, between the hydroxyl O(7) atom and the keto O(2) atom is also present {O(7)...O(2ⁱⁱⁱ) = 2.710 (3), O(7)—H = 0.94 Å, O(7)—H(7)...O(2ⁱⁱⁱ) = 177.7 (2)° [symmetry code: (iii) $-x + 1, y + \frac{1}{2}, -z + 1$] [see, for example, Subramanian, Sivakumar, Natarajan & Parthasarathy (1990) and Ueno & Saito (1976, 1977)]}.

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Trihydrate Structure of a Multisubstrate Inhibitor of L-DOPA Decarboxylase*

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Abstract. C₁₇H₁₈N₂O₆·3H₂O, $M_r = 400.4$, monoclinic, $P2_1$, $a = 4.872$ (1), $b = 17.824$ (2), $c = 11.149$ (2) Å, $\beta = 107.09$ (1)°, $V = 925.4$ (3) Å³, $Z = 2$, $D_m(\text{floatation}) = 1.44$ (1), $D_x = 1.437$ Mg m⁻³, $F(000) = 424$, $\lambda(\text{Cu } K\alpha) = 1.5418$ Å, $\mu = 0.90$ mm⁻¹, $T = 289$ (1) K. Final $R = 0.062$ for 1096 observed

* (1*S*,3*R*)-6,7-Dihydroxy-1-(3-hydroxy-5-hydroxymethyl-2-methylpyridin-4-yl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid trihydrate.

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data. The bridged diphenyl moiety comprising rings *A* and *C* linked through C(1) has a twist conformation, with the hydroxymethyl substituent at C(5') and the phenolic oxygen at C(3') in *distal* and *proximal* orientations respectively. The hydroxypyridine moiety is in the 1,3-dipolar ionic form and the isoquinoline ring nitrogen, N(2), is protonated with ionization at the carboxylate group.

Introduction. In the search for specific reversible inhibitors of L-DOPA decarboxylase (EC4.1.1.38) we

have utilized the multisubstrate concept (Andrews, Iskander, Jones & Winkler, 1982, 1988). The interest in finding inhibitors of this enzyme is justified by its important catalytic role in the synthesis of the known neurotransmitters dopamine, noradrenaline and serotonin in both central and peripheral neurons (Pletscher, Gey & Burkard, 1966). Several such inhibitors including (I) have been synthesized and biologically evaluated against the activity of the target enzyme (Brinkworth, Iles, Iskander & Andrews, 1988). Although the relative molecular structure of (I) has been previously established (Bringmann & Schneider, 1986) and its absolute structure assigned by comparison with that of D-DOPA (II), the X-ray structure reported here has defined the conformational detail in the molecule of (I).

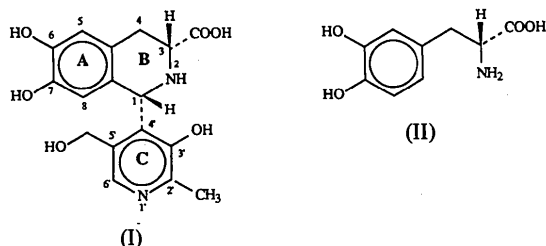


Table 1. Final atomic coordinates ($\times 10^4$) and equivalent isotropic temperature factors for the non-H atoms with e.s.d.'s in parentheses

$$B_{eq} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	$B_{eq}(\text{\AA}^2)$
C(1)	-280 (17)	3610 (6)	10997 (6)	1.5 (1)*
N(2)	-525 (13)	4379 (5)	11512 (6)	1.7 (1)
C(3)	-1976 (17)	4930 (6)	10512 (6)	1.6 (1)
C(4)	-226 (20)	5033 (6)	9602 (6)	2.6 (2)
C(4a)	846 (17)	4304 (6)	9213 (6)	2.1 (1)
C(5)	1918 (17)	4298 (6)	8172 (6)	2.1 (1)
C(6)	3122 (18)	3656 (6)	7832 (6)	2.3 (2)
O(6)	4299 (13)	3637 (5)	6881 (5)	3.2 (1)
C(7)	3113 (17)	2990 (6)	8510 (6)	2.4 (2)
O(7)	4242 (13)	2356 (5)	8148 (6)	3.6 (1)
C(8)	1976 (18)	2989	9507 (6)	2.3 (2)
C(8a)	873 (16)	3644 (6)	9893 (6)	1.7 (1)
N(1)	4716 (15)	2385 (6)	14153 (6)	2.7 (1)
C(2)	5732 (18)	3066 (6)	13940 (6)	2.4 (2)
C(3')	4183 (17)	3476 (6)	12862 (6)	2.1 (2)
O(3')	5080 (12)	4126 (5)	12615 (5)	2.3 (1)
C(4')	1573 (16)	3149 (6)	12089 (6)	1.7 (1)
C(5')	719 (17)	2429 (6)	12362 (6)	2.2 (1)
C(6')	2372 (18)	2056 (6)	13390 (6)	2.4 (2)
C(9)	-2173 (17)	5687 (6)	11169 (6)	2.1 (2)*
O(9a)	-760 (13)	5738 (6)	12275 (6)	3.6 (1)
O(9b)	-3718 (13)	6170 (5)	10475 (5)	3.4 (1)
C(10)	-1930 (21)	2067 (6)	11493 (9)	3.2 (2)
O(10)	-2458 (13)	1376 (6)	11967 (6)	4.1 (1)
C(11)	8392 (20)	3366 (6)	14881 (8)	3.4 (2)
OW(1)	3283 (17)	6741 (6)	3565 (6)	5.6 (2)
OW(2)	2777 (18)	332 (6)	5583 (6)	6.7 (2)
OW(3)	3361 (23)	4974 (6)	5655 (10)	9.7 (3)

* Isotropic temperature factors.

Experimental. (I) was prepared by condensation of D-DOPA (II) with pyridoxal phosphate via a Pictet-Spengler-type reaction (Schöpf & Bayerle, 1934) and formed cream-coloured platelets from methanol (dec. 522 K). A crystal ca $0.25 \times 0.25 \times 0.04$ mm aligned on a Rigaku-AFC diffractometer; cell parameters determined by least squares for 25 strong reflections ($31^\circ < 2\theta < 81^\circ$); Cu $K\alpha$ radiation (graphite-crystal monochromator, $\lambda = 1.5418 \text{ \AA}$); ω - 2θ scan, scan rate 2° min^{-1} , scan range ($\Delta\omega$) $(1.2 + 0.5 \tan\theta)^\circ$, 10 s stationary background counts; three standard reflections monitored every 50 reflections, no significant variation in intensity; data to $2\theta_{\text{max}} = 130^\circ$; 1414 unique data ($h - 5$ to 5 , $k 0$ to 20 , $l 0$ to 13) for which 1096 with $I_o > \sigma I_o$ for refinement; corrections for Lorentz and polarization and analytical corrections for absorption (transmission factors 0.857 to 0.968) with *SHELX76* (Sheldrick, 1976). Structure solved by direct methods; H atoms bonded to N(1'), O(6) and O(10) included at sites located on difference maps; H atom bonded to O(7) and those of water molecules not located; remaining H atoms included at idealized positions (C—H 1.08 , N—H 0.97 \AA). Full-matrix least-squares refinement, with anisotropic temperature factors given to the C, N and O atoms, excepting C(1) and C(9) which were given isotropic temperature factors,* and an overall iso-

tropic $B = 5.6 (6) \text{ \AA}^2$ for H atoms, converged at $R 0.062$, $wR 0.061$, $S 1.22$ (244 parameters varied); function minimized $\sum w(|F_o| - |F_c|)^2$, with weights $(\sigma^2 |F_o| + 0.001 |F|^2)^{-1}$; an isotropic extinction parameter of the form $F_c = F[1 - (4.0 \times 10^{-6} |F|^2 / \sin\theta)]$ was applied to the calculated structure amplitudes. At convergence $(\Delta/\sigma)_{\text{max}} 0.04$, $(\Delta\rho)_{\text{max}} + 0.31$ and $(\Delta\rho)_{\text{min}} - 0.27 \text{ e \AA}^{-3}$. Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). Figures prepared from the output of *ORTEPII* (Johnson, 1976). Major calculations made with *SHELX76* (Sheldrick, 1976) 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 the molecular geometry is given in Table 2.

The absolute molecular structure of (I) is shown in Fig. 1. The bridged diphenyl moiety comprising rings

* 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 52822 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

* These atoms would not refine meaningfully with anisotropic thermal parameters.

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

C(1)—N(2)	1.504 (13)	N(1')—C(2')	1.358 (16)
C(1)—C(4')	1.525 (11)	N(1')—C(6')	1.342 (11)
C(1)—C(8a)	1.497 (12)	C(2')—C(3')	1.419 (12)
N(2)—C(3)	1.498 (11)	C(2')—C(11)	1.506 (12)
C(3)—C(4)	1.516 (14)	C(3')—O(3')	1.297 (13)
C(3)—C(9)	1.552 (14)	C(3')—C(4')	1.434 (11)
C(4)—C(4a)	1.511 (15)	C(4')—C(5')	1.410 (15)
C(4a)—C(5)	1.406 (13)	C(5')—C(6')	1.364 (11)
C(4a)—C(8a)	1.397 (14)	C(5')—C(10)	1.512 (12)
C(5)—C(6)	1.388 (15)	C(8)—C(8a)	1.404 (11)
C(6)—O(6)	1.346 (11)	C(9)—O(9a)	1.226 (9)
C(6)—C(7)	1.408 (15)	C(9)—O(9b)	1.251 (11)
C(7)—O(7)	1.369 (13)	C(10)—O(10)	1.394 (15)
C(7)—C(8)	1.380 (13)		
N(2)—C(1)—C(8a)	111.6 (6)	C(1)—C(8a)—C(8)	119.2 (6)
N(2)—C(1)—C(4')	106.3 (6)	C(4a)—C(8a)—C(8)	118.5 (6)
C(8a)—C(1)—C(4')	113.6 (6)	C(2')—N(1')—C(6')	124.5 (7)
C(1)—N(2)—C(3)	112.7 (6)	N(1')—C(2')—C(3')	118.5 (7)
C(4)—C(3)—N(2)	110.0 (6)	N(1')—C(2')—C(11)	118.6 (7)
N(2)—C(3)—C(9)	107.5 (6)	C(3')—C(2')—C(11)	122.8 (7)
C(4)—C(3)—C(9)	109.6 (7)	C(2')—C(3')—O(3')	120.8 (7)
C(3)—C(4)—C(4a)	113.4 (7)	C(2')—C(3')—C(4')	117.2 (7)
C(4)—C(4a)—C(5)	119.2 (7)	O(3')—C(3')—C(4')	122.0 (6)
C(4)—C(4a)—C(8a)	121.2 (7)	C(1)—C(4')—C(3')	118.3 (6)
C(5)—C(4a)—C(8a)	119.7 (7)	C(1)—C(4')—C(5')	121.3 (6)
C(4a)—C(5)—C(6)	121.4 (7)	C(3')—C(4')—C(5')	120.4 (7)
C(5)—C(6)—O(6)	123.2 (7)	C(4')—C(5')—C(6')	119.1 (7)
C(5)—C(6)—C(7)	118.7 (7)	C(4')—C(5')—C(10)	120.0 (7)
O(6)—C(6)—C(7)	118.1 (7)	C(6)—C(5')—C(10)	120.8 (7)
C(6)—C(7)—O(7)	118.2 (7)	N(1')—C(6')—C(5')	120.1 (7)
C(6)—C(7)—C(8)	119.9 (7)	C(3)—C(9)—O(9a)	116.4 (7)
O(7)—C(7)—C(8)	121.9 (6)	C(3)—C(9)—O(9b)	114.6 (6)
C(7)—C(8)—C(8a)	121.7 (6)	O(9a)—C(9)—O(9b)	129.0 (7)
C(1)—C(8a)—C(4a)	122.3 (7)	C(5')—C(10)—O(10)	110.6 (7)
C(1)—N(2)—C(3)—C(9)	178	C(8a)—C(1)—C(4')—C(3')	76
C(1)—N(2)—C(3)—C(4)	-63	N(2)—C(1)—C(4')—C(3')	-47
N(2)—C(3)—C(4)—C(4a)	45	N(2)—C(1)—C(4')—C(5')	131
C(4a)—C(4)—C(3)—C(9)	163	C(8)—C(8a)—C(1)—C(4')	43
C(4)—C(3)—C(9)—O(9a)	-108	O(10)—C(10)—C(5')—C(4')	-177

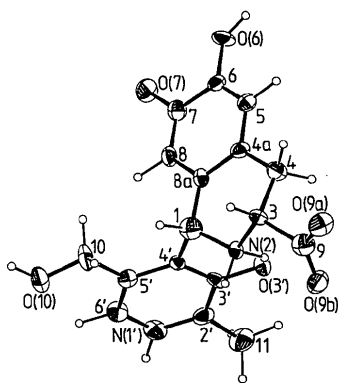


Fig. 1. A perspective view of the molecule with thermal ellipsoids scaled to 50% probability. The carbons are denoted by numerals only, and hydrogens are included as spheres of arbitrary radius.

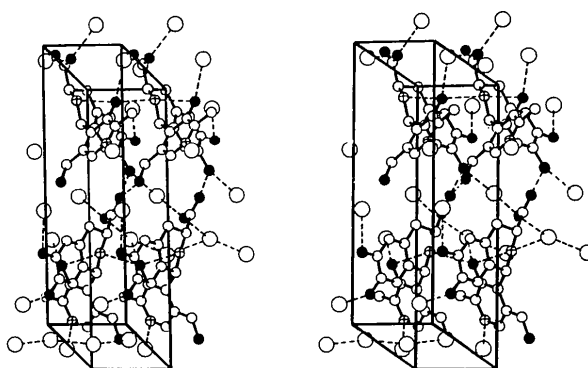
A and *C* linked through *C*(1) has a twist conformation with the hydroxymethyl substituent at *C*(5') in the *distal* orientation and the phenolic oxygen at *C*(3') *proximal*. The torsion angles *C*(8a)—*C*(1)—*C*(4')—*C*(3') and *C*(8)—*C*(8a)—*C*(1)—*C*(4') have the

Table 3. Hydrogen-bonding dimensions (Å, °) in $C_{17}H_{18}N_2O_6 \cdot 3H_2O$

<i>X</i> — <i>H</i> ... <i>Y</i>	<i>X</i> ... <i>Y</i>	<i>H</i> ... <i>Y</i>	<i>X</i> — <i>H</i>	<i>X</i> — <i>H</i> ... <i>Y</i>
N(1')—H(1')...O <i>W</i> (1)	2.70 (1)	1.87	0.93	147
N(2)—H(2a)...O(3')*	2.68 (1)	1.90	0.97†	136
N(2)—H(2b)...O(3') [†]	2.80 (1)	1.86	0.97†	162
O(6)—H(O6)...O <i>W</i> (3)	2.72 (1)	1.92	0.89	149
O(10)—H(O10)...O(9b) ⁱⁱ	2.84 (1)	1.98	1.08	126
O(7)...O(9b) ⁱⁱⁱ	2.67 (1)			
O <i>W</i> (2)...O(9a) ⁱⁱⁱ	2.93 (1)			
O <i>W</i> (1)...O(7) ^{iv}	2.77 (1)			
O <i>W</i> (1)...O <i>W</i> (3) ^v	2.74 (1)			
O <i>W</i> (2)...O(3') ^{vi}	2.92 (1)			
O <i>W</i> (3)...O <i>W</i> (2) ^{vii}	2.97 (1)			
O <i>W</i> (3)...O <i>W</i> (2) ^{viii}	2.72 (2)			

Symmetry codes: (i) $-1+x, y, z$; (ii) $-1-x, -\frac{1}{2}+y, 2-z$; (iii) $-x, -\frac{1}{2}+y, 2-z$; (iv) $x, y, 1+z$; (v) $-x, -\frac{1}{2}+y, 3-z$; (vi) $1-x, -\frac{1}{2}+y, 2-z$; (vii) $-x, \frac{1}{2}+y, 1-z$; (viii) $1-x, \frac{1}{2}+y, 1-z$.

* Intramolecular interaction.
† N—H bond distance constrained.

Fig. 2. Stereoview of the crystal packing. Direction of projection *c*, the *b* axis is vertical. O and N atoms in the molecule shaded, water oxygens larger and unshaded.

respective values of +76 (1) and +43 (1)°, both having the same sign as is generally observed for bridged diphenyls (Van der Heijden, Griffith, Chandler & Robertson, 1975). Ring *B* is in a half-chair form with atoms N(2), C(1), C(8a), C(4a) and C(4) lying close to a plane (r.m.s.d. 0.09 Å) with C(1) at 0.14 (1) Å and C(3) at 0.60 (1) Å from the plane. The hydroxypyridine moiety of ring *C* is in the 1,3-dipolar ionic form, and the isoquinoline ring nitrogen of ring *B*, N(2), is protonated with ionization at the carboxylate group. There is one intramolecular hydrogen bond in the structure in which N(2) is the donor atom in an interaction with the phenolic oxygen, O(3'); the N(2)...O(3'), N(2)—H(2a) and H(2a)...O(3') spacings are 2.68 (1), 0.97 and 1.90 Å respectively with the N(2)—H(2a)...O(3') angle 136°. All bond lengths and angles are normal (see Table 2).

The crystal packing is illustrated in Fig. 2. Inter-molecular hydrogen bonds link the inhibitor and water molecules into a three-dimensional network.

The O...O spacings range from 2.67 (1) to 2.97 (1) Å and the N(1)...O*W* (1) and N(2)...O(3') spacings have the respective values of 2.70 (1) and 2.80 (1) Å (see Table 3).

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Structure of a Photodimer of 3-Acetoxy-2-inden-1-one: 9,10-Dioxoindano[2',3':4,3]cyclobuta[1,2-*b*]indan-4b,4c-diyl Diacetate

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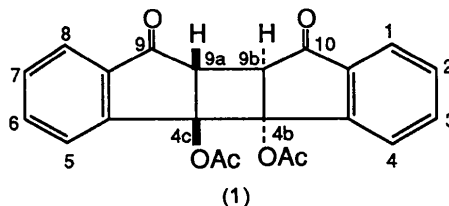
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Abstract. C₂₂H₁₆O₆, *M_r* = 376.37, monoclinic, *P*2₁/*c*, *a* = 9.555 (3), *b* = 15.664 (2), *c* = 12.300 (4) Å, β = 100.08 (2)°, *V* = 1812.5 (5) Å³, *Z* = 4, *D_x* = 1.379 g cm⁻³, λ(Cu Kα) = 1.5418 Å, μ = 8.0 cm⁻¹, *F*(000) = 784, room temperature, *R* = 0.047, *wR* = 0.064 for 3203 observed reflections [*I* > 3σ(*I*)]. The molecule exists as the *syn-trans* isomer in the crystal. The crystal structure exhibits a number of C—H...O intermolecular contacts.

Introduction. In connection with the synthesis of radermachol (Joshi, Gawad, Pelletier, Kartha & Bhandary, 1984), we carried out a photochemical reaction between 3-acetoxy-2-inden-1-one and 1,1,4,4-tetramethoxy-1,4-dihydronaphthalene. The photochemical reaction of enones with olefins has been investigated by several workers and fairly good yields of the photoaddition product have been obtained (Bryce-Smith & Gilbert, 1964; Bärltrop & Hesp, 1967; Pappas & Portnoy, 1970; Maruyama, Otsuki & Naruta, 1973; Otsuki, 1976). However, in the present case, the indenone being highly reactive, rapidly dimerized to give a compound C₂₂H₁₆O₆ (1);

the same compound was also obtained by photo reaction of the indenone. Four isomeric structures of the truxenone derivatives (*syn-cis*, *syn-trans*, *anti-cis* and *anti-trans*) are possible for the dimer. It was difficult to make a choice among the four, based only on the ¹H, ¹³C and mass spectral evidence. The correct structure was therefore determined by X-ray diffraction and is reported here.



Experimental. 3-Acetoxy-2-inden-1-one was prepared by following a reported procedure (Sraga & Hunciar, 1986). The dimer was obtained by irradiating a solution of the indenone (100 mg) in benzene (400 ml) at 285 K for two hours under nitrogen with a medium pressure mercury lamp. The solvent was removed and the product crystallized from benzene to afford the dimer (63 mg). This was recrystallized

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