quadrangular conformation, with the protonated N atoms located in corner positions (see Fig. 1).

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Structure of a Melanin Precursor: 1-Methylindole-5,6-diol

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Abstract. $C_9H_9NO_2$, $M_r = 163{\cdot}18$, rhombohedral, $R3c$, $a = 12{\cdot}814\,(4)$ Å, $\alpha = 114{\cdot}59\,(2)^\circ$, $V = 1220{\cdot}4$ Å^3, $Z = 6$, $D_x = 1{\cdot}332$ Mg m^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71073$ Å, $\mu = 0{\cdot}089$ mm^{-1}, $F(000) = 516$, $T = 293\,(1)$ K. $R = 0{\cdot}027$ for 410 observed reflections with $I > 3\sigma(I)$. The C—O distances in the catechol [1·396 (4) and 1·388 (5) Å] are identical. The indole moiety is planar with O(1) 0·139 (2) Å out of the plane of the indole moiety. The structure is stabilized by two short intermolecular distances O(1)···H(O1) 1·80 and O(1)···H(O2) 1·73 Å and there is a short intramolecular contact O(2)···H(O1) of 2·03 Å.

Experimental. A small crystal of approximate dimensions 0·16 × 0·17 × 0·32 mm was obtained by cutting a long needle. Accurate cell dimensions and a crystal orientation matrix were determined on an Enraf–Nonius CAD-4 diffractometer by a least-squares refinement of the setting angles of 25 reflections with θ in the range 10–15°. Intensity data were collected by the $\omega/2\theta$ scan method and variable scan speed (0·55–3·5° min^{-1}) using graphite-monochromatized radiation in the range $2 < \theta < 25^\circ$. The intensities of three standard reflections, monitored at regular intervals, did not decrease over the course of the data collection. Intensities of 790 reflections were measured, of which 410 had $I > 3\sigma(I)$, and were used in the structure solution and refinement. Data were corrected for Lorentz and polarization factors; absorption correction was deemed unnecessary.

The structure was solved by direct methods using *MULTAN*82 (Main, Fiske, Hull, Lessinger, Germain, Delcercq & Woolfson, 1982). Refinement of the structure was by full-matrix least-squares calculations on F's, initially with isotropic and finally with anisotropic temperature factors for the non-H atoms. At an intermediate stage in the refinement, a difference map revealed all H atoms which were included in the subsequent cycles at fixed positions and with an overall isotropic thermal parameter. Refinement converged with $R = 0{\cdot}027$ and $wR = 0{\cdot}030$; maximum shift/e.s.d. < 0·02, $S = 1{\cdot}008$, and $w = 1/(\sigma^2F + 0{\cdot}040F^2)$. Scattering factors were those of Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965). A difference map calculated at the conclusion of the refinement had no chemically significant features with electron density ±0·10 e Å^{-3}. All computer programs used are part of the Enraf–

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Table 1. *Final fractional coordinates and equivalent isotropic thermal parameters* (Å^2), *with e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}[a^2B_{11} + b^2B_{22} + c^2B_{33} + ab(\cos\gamma)B_{12} + ac(\cos\beta)B_{13} + bc(\cos\alpha)B_{23}]$.

	x	y	z	B_{eq}
O(1)	0·8095*	0·7166 (2)	0·8757 (2)	4·30 (7)
O(2)	0·4988 (2)	0·5508 (2)	0·7020 (2)	4·90 (7)
N	0·4074 (3)	0·0966 (2)	0·6058 (3)	4·89 (9)
C(1)	0·7674 (3)	0·4995 (3)	0·8436 (3)	4·3 (1)
C(2)	0·7069 (3)	0·5615 (3)	0·8136 (3)	3·5 (1)
C(3)	0·5418 (3)	0·4709 (3)	0·7164 (3)	3·7 (1)
C(4)	0·4291 (3)	0·3137 (3)	0·6408 (3)	4·0 (1)
C(5)	0·4892 (3)	0·2481 (3)	0·6660 (3)	3·9 (1)
C(6)	0·6576 (3)	0·3405 (3)	0·7699 (3)	4·2 (1)
C(7)	0·6724 (3)	0·2348 (3)	0·7664 (3)	5·9 (1)
C(8)	0·5184 (4)	0·0895 (3)	0·6654 (4)	6·3 (1)
C(9)	0·2322 (5)	−0·0357 (4)	0·4918 (4)	6·8 (2)

* Fixed to define the origin.

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

O(1)	C(2)	1·396 (4)	C(2)	C(3)	1·391 (4)
O(2)	C(3)	1·388 (5)	C(3)	C(4)	1·368 (4)
N	C(5)	1·360 (4)	C(4)	C(5)	1·401 (6)
N	C(8)	1·370 (6)	C(5)	C(6)	1·415 (4)
N	C(9)	1·446 (4)	C(6)	C(7)	1·429 (7)
C(1)	C(2)	1·379 (6)	C(7)	C(8)	1·359 (5)
C(1)	C(6)	1·390 (5)			

C(5)	N	C(8)	108·3 (3)	C(3)	C(4)	C(5)	116·3 (3)
C(5)	N	C(9)	125·3 (4)	N	C(5)	C(4)	129·5 (3)
C(8)	N	C(9)	126·4 (3)	N	C(5)	C(6)	108·1 (4)
C(2)	C(1)	C(6)	118·1 (3)	C(4)	C(5)	C(6)	122·4 (3)
O(1)	C(2)	C(1)	120·7 (2)	C(1)	C(6)	C(5)	119·3 (4)
O(1)	C(2)	C(3)	117·6 (3)	C(1)	C(6)	C(7)	134·1 (3)
C(1)	C(2)	C(3)	121·7 (3)	C(5)	C(6)	C(7)	106·6 (3)
O(2)	C(3)	C(2)	115·7 (3)	C(6)	C(7)	C(8)	106·2 (4)
O(2)	C(3)	C(4)	122·1 (3)	N	C(8)	C(7)	110·9 (4)
C(2)	C(3)	C(4)	122·2 (4)				

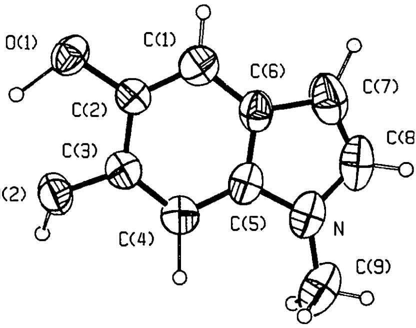

Fig. 1. Molecular structure of the title compound with the atomic numbering scheme.

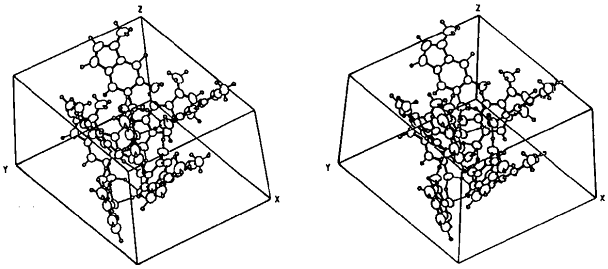

Fig. 2. Stereoview of the unit cell showing hydrogen bonds.

Nonius *SDP* (B. A. Frenz & Associates Inc., 1985), and the figures were plotted using the *ORTEP*II (Johnson, 1976) program.

The final fractional coordinates are given in Table 1* and bond distances and angles for non-H atoms are in Table 2. The molecular structure with our numbering scheme is depicted in Fig. 1. Fig. 2 shows the crystal packing.

Related literature. Structures of indole (Roychowdhury & Basak, 1975), 3*H*-indol-5-ol (Bocelli & Grenier-Loustalot, 1982), 5,6-dimethoxyindole (Shoja, 1988), 4-trimethylsilylindole (Barrett, Dauzonne & Williams, 1982), dimethyl 1-acetyl-6-hydroxyindole-4,5-dicarboxylate (Sivý, Koreň, Valach, Krutošíková & Pavelčík, 1988), and a closely related compound, 7-iodoadrenochrome (Opheim, 1979) have been reported.

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* Lists of structure amplitudes, anisotropic temperature factors, H-atom positions, molecular dimensions involving H atoms, and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52231 (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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Structure of Diethyl 4-Ethoxycarbonyl-3,4-dihydrobenzo[*f*]quinoline-3-phosphonate

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Abstract. $C_{20}H_{24}NO_5P$, $M_r = 389{\cdot}40$, monoclinic, $P2_1/a$, $a = 15{\cdot}332\ (3)$, $b = 10{\cdot}603\ (6)$, $c = 12{\cdot}442\ (6)$ Å, $\beta = 100{\cdot}89\ (3)°$, $V = 1986\ (1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}30$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å, $\mu = 1{\cdot}84$ cm^{-1}, $F(000) = 824$, room temperature, $R = 0{\cdot}059$ for 2108 observed reflections [$F_o > 3\sigma(F_o)$]. Out of 11 C—C bonds of the biphenyl ring, four bonds (1·35–1·38 Å) are significantly shorter than the others (1·40–1·43 Å). Two P—O single bonds are 1·564 (4) and 1·560 (4) Å in length, and the P—O double-bond length is 1·454 (4) Å.

Experimental. Title compound prepared according to the literature (Takeuchi, Shibata & Hamada, 1984). Colorless crystals obtained from ethanol solution. Crystal of dimensions 0·3 × 0·2 × 0·2 mm, Rigaku AFC-1 rotating-anode four-circle diffractometer, graphite-monochromatized Mo $K\alpha$ radiation. Cell dimensions determined from 16 2θ angles in the range $17 < 2\theta < 23°$. Intensities collected to $\sin\theta/\lambda =$

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{4}{3}[B_{11}a^2 + B_{22}b^2 + B_{33}c^2 + abB_{12}(\cos\gamma) + acB_{13}(\cos\beta) + bcB_{23}(\cos\alpha)].$$

	x	y	z	B_{eq}
P	0·5962 (1)	0·8906 (1)	0·1953 (1)	4·6 (0)
N	0·7481 (3)	0·7466 (3)	0·2224 (3)	4·3 (1)
O1	0·6079 (2)	0·8781 (3)	0·3226 (2)	5·2 (1)
O2	0·5597 (3)	1·0084 (3)	0·1463 (3)	6·8 (1)
O3	0·5422 (2)	0·7693 (3)	0·1552 (2)	5·8 (1)
O4	0·7216 (3)	0·6507 (4)	0·0566 (2)	6·8 (1)
O5	0·8056 (2)	0·5560 (3)	0·2010 (2)	5·4 (1)
C1	0·7090 (3)	0·8638 (4)	0·1737 (3)	4·7 (1)
C2	0·7684 (3)	0·9730 (5)	0·2099 (4)	5·0 (1)
C3	0·8237 (3)	0·9699 (4)	0·3063 (4)	4·8 (1)
C4	0·8246 (3)	0·8616 (4)	0·3794 (3)	3·8 (1)
C5	0·8607 (3)	0·8687 (4)	0·4942 (3)	3·8 (1)
C6	0·9025 (3)	0·9773 (5)	0·5451 (4)	5·0 (1)
C7	0·9369 (4)	0·9797 (5)	0·6543 (4)	6·1 (2)
C8	0·9317 (4)	0·8741 (6)	0·7198 (4)	6·4 (2)
C9	0·8915 (4)	0·7688 (5)	0·6748 (4)	5·5 (1)
C10	0·8540 (3)	0·7626 (4)	0·5607 (3)	4·1 (1)
C11	0·8130 (3)	0·6513 (4)	0·5125 (3)	4·3 (1)
C12	0·7797 (3)	0·6448 (4)	0·4034 (3)	4·0 (1)
C13	0·7872 (3)	0·7498 (4)	0·3367 (3)	3·5 (1)
C14	0·5358 (4)	0·8644 (7)	0·3794 (5)	7·5 (2)
C15	0·5730 (4)	0·8440 (5)	0·4958 (5)	7·1 (2)
C16	0·4985 (4)	0·7545 (6)	0·0410 (4)	7·4 (2)
C17	0·4262 (5)	0·6682 (11)	0·0347 (6)	14·4 (4)
C18	0·7558 (3)	0·6491 (5)	0·1520 (4)	5·0 (1)
C19	0·8167 (4)	0·4481 (5)	0·1311 (5)	7·0 (2)
C20	0·8487 (5)	0·3426 (6)	0·1990 (5)	8·6 (2)

Table 2 *Bond lengths* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

P—O1	1·566 (4)	P—O2	1·454 (4)	P—O3	1·559 (4)
P—C1	1·822 (5)	N—C1	1·460 (6)	N—C13	1·436 (6)
O1—C14	1·427 (8)	O3—C16	1·460 (7)	O4—C18	1·203 (6)
O5—C18	1·324 (6)	O5—C19	1·466 (8)	C2—C3	1·332 (7)
C3—C4	1·464 (7)	C4—C5	1·433 (6)	C4—C13	1·379 (6)
C5—C6	1·409 (6)	C5—C10	1·412 (6)	C6—C7	1·362 (7)
C7—C8	1·396 (8)	C8—C9	1·346 (8)	C9—C10	1·429 (7)
C10—C11	1·416 (7)	C11—C12	1·359 (7)	C12—C13	1·406 (6)
C14—C15	1·468 (10)	C16—C17	1·428 (13)	C19—C20	1·431 (10)

O1—P—O2	117·2 (2)	O1—P—O3	101·9 (2)
O1—P—C1	101·9 (2)	O2—P—O3	115·8 (2)
O2—P—C1	111·9 (2)	O3—P—C1	106·6 (2)
C1—N—C13	116·9 (4)	C1—N—C18	117·0 (4)
C13—N—C18	125·4 (4)	P—O1—C14	124·0 (4)
P—O3—C16	121·2 (4)	C18—O5—C19	115·5 (4)
P—C1—N	113·5 (3)	P—C1—C2	112·2 (4)
N—C1—C2	110·9 (4)	C1—C2—C3	120·1 (5)
C2—C3—C4	120·6 (5)	C3—C4—C5	122·3 (4)
C3—C4—C13	118·8 (4)	C5—C4—C13	118·9 (4)
C4—C5—C6	123·2 (4)	C4—C5—C10	119·0 (4)
C6—C5—C10	117·7 (4)	C5—C6—C7	121·4 (5)
C6—C7—C8	120·9 (5)	C7—C8—C9	119·6 (6)
C8—C9—C10	121·2 (5)	C5—C10—C9	119·1 (4)
C5—C10—C11	119·4 (4)	C9—C10—C11	121·5 (4)
C10—C11—C12	121·2 (4)	C11—C12—C13	119·5 (4)
N—C13—C4	117·8 (4)	N—C13—C12	120·1 (4)
C4—C13—C12	121·9 (4)	O1—C14—C15	108·1 (5)
O3—C16—C17	109·3 (7)	N—C18—O4	122·9 (5)
N—C18—O5	112·3 (4)	O4—C18—O5	124·8 (5)
O5—C19—C20	109·0 (6)		

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