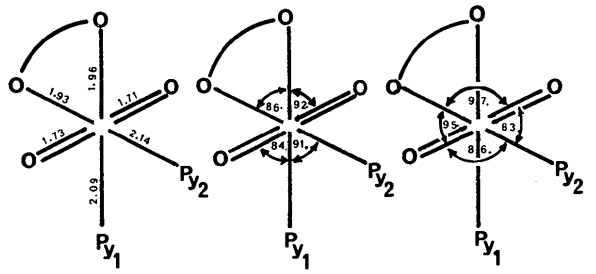

Fig. 3. Distances and angles around the Os atom.

spatial surrounding of this atom to obtain information about the activated complex of this addition.

The 0*kl* projection of the molecule displayed in Fig. 2 indicates that both pyridine rings are *trans* to the O–Os bonds of the benzanthracene moiety. Distances and angles around the Os atom are given in Fig. 3.

Both Figs. 2 and 3 reveal that important distortion from idealized octahedral geometry occurs around the Os atom.

As reported in other 6,7-dihydro compounds of benzanthracene (Glusker, Carrel, Zacharias & Harvey, 1974) the aromatic parts of the molecule are folded in two parts about the saturated *C* ring by an angle of 20°.

The toluene molecule was found to be more thermally agitated than the associated Os complex and some difficulties have been encountered in determining accurately the coordinates of its methyl group.

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Cinnzeylanine, A New Pentacyclic Diterpene Acetate from *Cinnamonum zeylanicum*

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(*Received* 23 *September* 1976; *accepted* 21 *October* 1976)

Abstract. $C_{22}H_{34}O_8$, M_r = 426·51; orthorhombic, $P2_12_12_1$, a = 12·195 (2), b = 13·476 (2), c = 12·891 (1) Å, Z = 4, V = 2118·6 (5) Å^3, D_x = 1·35, D_m = 1·34 g cm^{-3} (flotation); λ(Mo $K\alpha$) = 0·71069 Å, μ(Mo $K\alpha$) = 1·371 cm^{-1}. The structure was solved by the direct method and refined by block-diagonal least squares. The final R value was 0·067 for 2442 reflexions. The skeleton of the compound is very similar to that of ryanodine [Wiesner, *Advanc. Org. Chem.* (1972), **8**, 295–316].

Introduction. Cinnzeylanine is a new compound isolated from the dried bark of *Cinnamonum zeylanicum* Nees as an insect-growth regulator (Isogai, Suzuki, Tamura, Murakoshi, Ohashi & Sasada, 1976). Prismatic crystals were obtained by recrystallization from ethyl acetate–benzene. Intensity data up to $2\theta \leq 55°$ were collected with a crystal, 0·2 × 0·5 × 0·5 mm, on a Rigaku four-circle diffractometer and Mo $K\alpha$ radiation monochromatized by graphite; an ω–2θ scan at 4° (2θ) min^{-1} was employed. A Lorentz–polarization

correction was made as usual. Structure factors for 2744 reflexions were obtained; 299 of these with $|F_o| < 3{\cdot}0(\sigma|F_o|)$ were considered as unobserved. The structure was solved by the direct method with the program *MULTAN* (Germain, Main & Woolfson, 1971) and refined by block-diagonal least squares with the modified *HBLS* program. The function minimized was $\Sigma w(|F_o| - |F_c|)^2$, where w is the weight as follows: $w = 0{\cdot}3$ for $|F_o| < 2{\cdot}57$ and $|F_o| > 25{\cdot}7$; $w = 1/(4{\cdot}8559 - 0{\cdot}49313F_o + 0{\cdot}01741F_o^2)$ for $2{\cdot}57 \leq |F_o| \leq 25{\cdot}7$. All H atoms were located in a difference map and their positions and isotropic temperature factors were also refined. Three strong reflexions were excluded because they seemed to suffer from secondary extinction. The final R was 0·067 for 2442 reflexions. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974).

The final positional and thermal parameters for the non-H and H atoms are listed in Tables 1 and 2 respectively.* Fig. 1 shows a schematic drawing of the present compound, with the atom-numbering system used.

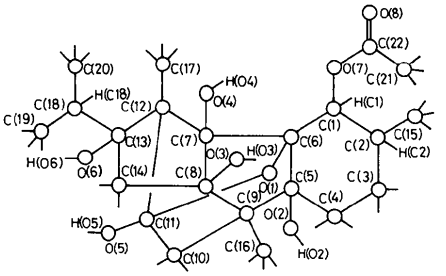

Fig. 1. A schematic drawing of cinnzeylanine with the atom-numbering system.

Discussion. In the crystal structure, shown in Fig. 2, a three-dimensional network is formed by weak hydrogen bonds, whose lengths and angles are given in Table 3. There is no intramolecular hydrogen bond. This is consistent with the observation of IR spectra in solution. The molecular structure is illustrated by the stereoscopic drawing (Fig. 3) produced with the *DCMS* program (Takenaka, 1972). The skeleton of this compound is very similar to that of ryanodine. From the

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32237 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Positional and thermal parameters for non-hydrogen atoms*

The parameters are multiplied by 10^4. The form of the anisotropic temperature factor is: $\exp(-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - \beta_{12}hk - \beta_{13}hl - \beta_{23}kl)$.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	2911 (3)	−1435 (3)	1203 (3)	49 (3)	42 (2)	41 (2)	−1 (4)	−2 (4)	−8 (4)
C(2)	2714 (4)	−2139 (3)	2122 (3)	75 (3)	40 (2)	49 (3)	2 (5)	−25 (5)	3 (4)
C(3)	1486 (4)	−2356 (3)	2252 (3)	79 (3)	45 (2)	51 (3)	−38 (5)	−8 (6)	13 (5)
C(4)	750 (3)	−1430 (3)	2269 (3)	56 (3)	53 (3)	55 (3)	−26 (5)	0 (5)	8 (5)
C(5)	1002 (3)	−781 (3)	1344 (3)	50 (3)	39 (2)	43 (2)	−1 (4)	8 (5)	−13 (5)
C(6)	2222 (3)	−502 (3)	1331 (3)	51 (3)	36 (2)	36 (2)	4 (4)	3 (4)	2 (4)
C(7)	2308 (3)	383 (3)	554 (3)	45 (3)	38 (2)	34 (2)	−1 (4)	−1 (4)	5 (4)
C(8)	1104 (3)	684 (3)	281 (3)	53 (3)	41 (2)	45 (2)	7 (4)	2 (5)	−7 (5)
C(9)	475 (3)	258 (3)	1230 (3)	45 (3)	43 (2)	45 (3)	1 (4)	−2 (5)	−6 (5)
C(10)	839 (3)	894 (3)	2166 (3)	48 (3)	41 (2)	40 (2)	2 (4)	24 (4)	−8 (4)
C(11)	2091 (3)	952 (3)	2240 (3)	55 (3)	36 (2)	40 (2)	1 (4)	6 (5)	0 (5)
C(12)	2679 (3)	1273 (3)	1226 (3)	46 (3)	37 (2)	38 (2)	−6 (4)	8 (4)	−6 (4)
C(13)	2206 (3)	2187 (3)	663 (3)	62 (3)	37 (2)	44 (2)	−11 (5)	22 (5)	3 (5)
C(14)	1103 (3)	1824 (3)	219 (3)	58 (3)	46 (2)	45 (2)	13 (5)	1 (5)	12 (5)
C(15)	3365 (4)	−3105 (3)	2008 (4)	102 (5)	51 (2)	96 (4)	10 (7)	9 (8)	47 (8)
C(16)	−771 (3)	231 (3)	1119 (3)	53 (3)	61 (3)	70 (3)	3 (5)	−4 (6)	−8 (6)
C(17)	3931 (2)	1288 (3)	1403 (3)	52 (3)	54 (2)	52 (2)	−12 (5)	5 (5)	−4 (5)
C(18)	2079 (4)	3158 (3)	1291 (3)	82 (4)	44 (2)	47 (3)	−3 (5)	23 (6)	0 (6)
C(19)	1504 (5)	3964 (3)	652 (4)	124 (5)	41 (3)	82 (4)	25 (6)	−3 (8)	−2 (8)
C(20)	3155 (4)	3576 (3)	1710 (4)	99 (4)	50 (3)	80 (4)	−15 (6)	−3 (7)	−33 (7)
C(21)	5858 (4)	−1271 (4)	552 (4)	63 (3)	65 (3)	86 (4)	5 (6)	13 (6)	−3 (6)
C(22)	4671 (3)	−1522 (3)	399 (4)	63 (3)	43 (2)	52 (3)	28 (5)	2 (5)	17 (5)
O(1)	2463 (2)	−67 (2)	2334 (2)	54 (2)	38 (1)	33 (1)	0 (3)	0 (3)	−3 (3)
O(2)	789 (2)	−1343 (2)	406 (2)	64 (2)	45 (2)	51 (2)	−17 (3)	−12 (3)	−13 (3)
O(3)	748 (4)	319 (2)	−693 (2)	76 (2)	44 (2)	46 (2)	1 (4)	−31 (3)	−10 (4)
O(4)	2959 (2)	234 (2)	−344 (2)	61 (2)	53 (3)	32 (1)	6 (3)	6 (3)	−5 (3)
O(5)	2459 (2)	1478 (2)	3096 (2)	67 (2)	52 (2)	37 (1)	−9 (4)	5 (3)	−14 (3)
O(6)	2927 (2)	2433 (2)	−201 (2)	78 (2)	48 (2)	49 (2)	0 (4)	35 (4)	8 (4)
O(7)	4069 (2)	−1174 (2)	1177 (2)	54 (2)	44 (4)	44 (2)	5 (3)	2 (3)	−7 (3)
O(8)	4319 (2)	−1992 (2)	−326 (2)	69 (2)	68 (2)	56 (2)	29 (4)	−3 (4)	−36 (4)

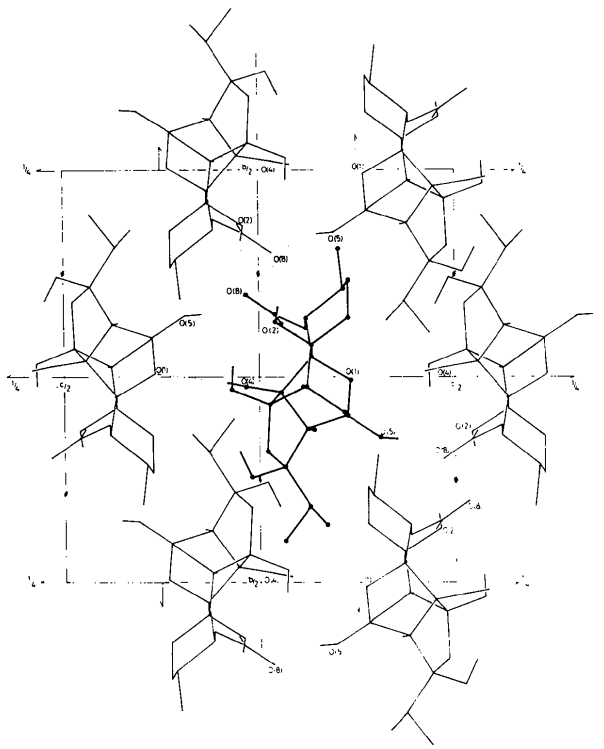

Fig. 2. The crystal structure projected along **a**, H atoms bonded to C atoms being excluded. The hydrogen bonds are represented by broken lines.

Table 2. *Positional* ($\times 10^3$) *and thermal parameters for hydrogen atoms*

	x	*y*	*z*	*B* (Å²)
H(C1)	2674 (2)	−1782 (2)	563 (2)	1·2 (6)
H(C2)	3010 (3)	−1777 (2)	2720 (2)	2·0 (7)
H(C31)	1232 (2)	−2741 (2)	1716 (2)	1·5 (7)
H(C32)	1399 (3)	−2749 (3)	2870 (3)	3·3 (8)
H(C41)	−21 (3)	−1592 (2)	2243 (2)	2·5 (8)
H(C42)	932 (3)	−1057 (2)	2907 (2)	2·2 (7)
H(C101)	595 (3)	610 (2)	2817 (2)	2·1 (7)
H(C102)	507 (3)	1509 (2)	2086 (2)	2·4 (7)
H(C141)	416 (8)	2079 (3)	642 (3)	3·2 (9)
H(C142)	1022 (3)	1965 (3)	−471 (2)	3·1 (8)
H(C151)	3125 (2)	−3390 (3)	1381 (3)	7·1 (13)
H(C152)	3246 (3)	−3523 (3)	2543 (3)	3·9 (9)
H(C153)	4181 (4)	−2942 (3)	1951 (4)	7·1 (13)
H(C161)	−1006 (4)	−137 (3)	573 (3)	5·7 (11)
H(C162)	−1031 (4)	51 (3)	1703 (4)	7·2 (13)
H(C163)	−1059 (3)	878 (3)	928 (3)	3·6 (9)
H(C171)	4191 (4)	748 (3)	1652 (3)	6·0 (12)
H(C172)	4278 (3)	1390 (3)	786 (3)	5·4 (11)
H(C173)	4153 (4)	1748 (3)	1874 (4)	7·1 (13)
H(C18)	1647 (3)	2972 (2)	1931 (3)	2·5 (7)
H(C191)	1466 (4)	4474 (3)	1086 (3)	6·2 (12)
H(C192)	681 (4)	3687 (4)	402 (4)	9·4 (15)
H(C193)	1756 (4)	3994 (4)	−51 (4)	8·7 (15)
H(C201)	3000 (4)	4202 (3)	2056 (3)	5·5 (11)
H(C202)	3510 (3)	3144 (3)	2291 (3)	5·4 (11)
H(C203)	3739 (4)	3581 (3)	1141 (3)	5·9 (11)
H(C211)	6193 (4)	−1154 (4)	−71 (4)	8·4 (14)
H(C212)	6225 (4)	−1833 (4)	825 (4)	7·6 (14)
H(C213)	5960 (4)	−697 (3)	1060 (4)	6·8 (13)
H(O2)	334 (4)	−1689 (3)	459 (4)	7·2 (14)
H(O3)	728 (3)	−232 (2)	−674 (2)	1·2 (6)
H(O4)	2652 (3)	148 (3)	−806 (2)	2·6 (8)
H(O5)	2004 (3)	1506 (3)	3543 (3)	4·3 (10)
H(O6)	3240 (4)	1885 (4)	−479 (4)	8·1 (14)

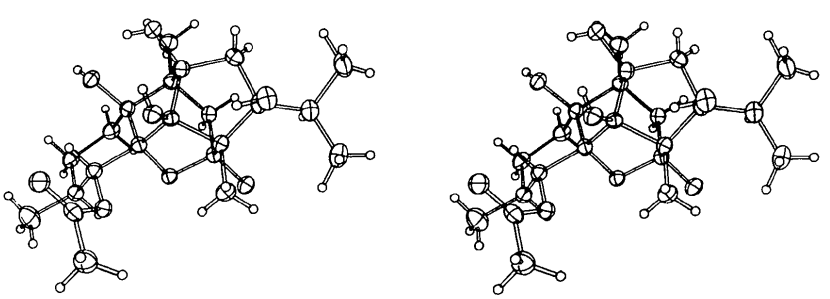

Fig. 3. Stereoscopic view with thermal ellipsoids at 30% probability.

Table 3. *Hydrogen-bond lengths and angles*

D	H	*A*	Position of acceptor atom	Distance (Å) *D*···*A*	H···*A*	Angle (°) *D*–H···*A*
O(2)	H(O2)	O(8)	$-\frac{1}{2}+x$, $-\frac{1}{2}-y$, $-z$	2·875 (4)	2·17 (5)	162 (5)
O(5)	H(O5)	O(8)	$\frac{1}{2}-x$, $-y$, $\frac{1}{2}+z$	3·053 (4)	2·27 (4)	165 (4)
O(4)	H(O4)	O(1)	$\frac{1}{2}-x$, $-y$, $-\frac{1}{2}+z$	3·045 (4)	2·40 (4)	151 (4)

Table 4. *Bond lengths* (Å)

Those for C–H are omitted.

C(1)–C(2)	1·536 (6)	C(1)–C(6)	1·521 (5)
C(1)–O(7)	1·456 (5)	C(2)–C(3)	1·535 (6)
C(2)–C(15)	1·533 (7)	C(3)–C(4)	1·538 (6)
C(4)–C(5)	1·510 (6)	C(5)–C(6)	1·534 (6)
C(5)–C(9)	1·549 (5)	C(5)–O(2)	1·450 (5)
C(6)–C(7)	1·560 (5)	C(6)–O(1)	1·450 (5)
C(7)–C(8)	1·565 (5)	C(7)–C(12)	1·546 (5)
C(7)–O(4)	1·418 (4)	C(8)–C(9)	1·553 (6)
C(8)–C(14)	1·537 (6)	C(8)–O(3)	1·417 (5)
C(9)–C(10)	1·547 (5)	C(9)–C(16)	1·527 (6)
C(10)–C(11)	1·532 (5)	C(11)–C(12)	1·552 (5)
C(11)–O(1)	1·452 (5)	C(11)–O(5)	1·387 (5)
C(12)–C(13)	1·542 (5)	C(12)–C(17)	1·544 (6)
C(13)–C(14)	1·541 (6)	C(13)–C(18)	1·547 (6)
C(13)–O(6)	1·457 (5)	C(18)–C(19)	1·533 (7)
C(18)–C(20)	1·526 (7)	C(21)–C(22)	1·499 (6)
C(22)–O(7)	1·328 (5)	C(22)–O(8)	1·207 (5)
O(2)–H(O2)	0·73 (5)	O(3)–H(O3)	0·74 (4)
O(4)–H(O4)	0·71 (4)	O(5)–H(O5)	0·80 (4)
O(6)–H(O6)	0·91 (5)		

$[\alpha]_D$ values of the derivatives of both compounds, the absolute configurations might be the same. Figs. 2 and 3 are drawn in a left-handed system in accordance with the configuration of ryanodine. Bond lengths and angles are shown in Tables 4 and 5 respectively. The dihedral angles C(22)–O(7)–C(1)–C(2) and O(6)–C(13)–C(18)–H(C18) are 111·0 and 174·1° respectively.

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Table 5. *Bonds angles* (°) *involving non-hydrogen atoms*

C(2)–C(1)–C(6)	109·9 (3)	O(5)–C(11)–O(1)	108·4 (3)	C(8)–C(7)–C(12)	101·5 (3)
C(6)–C(1)–O(7)	109·8 (3)	C(7)–C(12)–C(13)	104·3 (3)	C(12)–C(7)–O(4)	113·8 (3)
C(1)–C(2)–C(15)	111·7 (4)	C(11)–C(12)–C(13)	116·5 (3)	C(7)–C(8)–C(14)	105·8 (3)
C(2)–C(3)–C(4)	114·6 (4)	C(13)–C(12)–C(17)	115·4 (3)	C(9)–C(8)–C(14)	114·2 (3)
C(4)–C(5)–C(6)	110·4 (3)	C(12)–C(13)–C(18)	117·8 (3)	C(14)–C(8)–O(3)	107·6 (3)
C(4)–C(5)–O(2)	108·7 (3)	C(14)–C(13)–C(18)	112·1 (3)	C(5)–C(9)–C(10)	107·9 (3)
C(6)–C(5)–O(2)	107·0 (3)	C(18)–C(13)–O(6)	105·5 (3)	C(8)–C(9)–C(10)	105·7 (3)
C(1)–C(6)–C(5)	109·5 (3)	C(13)–C(18)–C(19)	111·3 (4)	C(10)–C(9)–C(16)	111·8 (3)
C(1)–C(6)–O(1)	108·6 (3)	C(19)–C(18)–C(20)	108·8 (4)	C(10)–C(11)–C(12)	115·1 (3)
C(5)–C(6)–O(1)	106·6 (3)	C(21)–C(22)–O(8)	124·2 (4)	C(10)–C(11)–O(1)	105·5 (3)
C(6)–C(7)–C(8)	106·2 (3)	C(6)–O(1)–C(11)	104·1 (3)	C(12)–C(11)–O(1)	101·0 (3)
C(6)–C(7)–O(4)	117·0 (3)	C(2)–C(1)–O(7)	108·6 (3)	C(7)–C(12)–C(11)	96·9 (3)
C(8)–C(7)–O(4)	112·2 (3)	C(1)–C(2)–C(3)	110·7 (4)	C(7)–C(12)–C(17)	112·5 (3)
C(7)–C(8)–C(9)	101·0 (3)	C(3)–C(2)–C(15)	110·7 (4)	C(11)–C(12)–C(17)	109·6 (3)
C(7)–C(8)–O(3)	113·4 (3)	C(3)–C(4)–C(5)	109·9 (3)	C(12)–C(13)–C(14)	104·3 (3)
C(9)–C(8)–O(3)	114·7 (3)	C(4)–C(5)–C(9)	121·0 (3)	C(12)–C(13)–O(6)	108·4 (3)
C(5)–C(9)–C(8)	101·8 (3)	C(6)–C(5)–C(9)	100·3 (3)	C(14)–C(13)–O(6)	108·4 (3)
C(5)–C(9)–C(16)	113·6 (3)	C(9)–C(5)–O(2)	108·6 (3)	C(8)–C(14)–C(13)	107·3 (3)
C(8)–C(9)–C(16)	115·2 (3)	C(1)–C(6)–C(7)	121·7 (3)	C(13)–C(18)–C(20)	114·3 (4)
C(9)–C(10)–C(11)	111·2 (3)	C(5)–C(6)–C(7)	105·1 (3)	C(21)–C(22)–O(7)	110·8 (4)
C(10)–C(11)–O(5)	113·4 (3)	C(7)–C(6)–O(1)	104·5 (3)	O(7)–C(22)–O(8)	124·9 (4)
C(12)–C(11)–O(5)	112·2 (3)	C(6)–C(7)–C(12)	104·7 (3)	C(1)–O(7)–C(22)	118·0 (3)