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Structure of Two Isomers of *cisoid*-4a,4b-*trans*-4b-2-(1,3-Dithiolan-2-yl)-1,2,3,4,4a,4b,5,6,7,8,8a,9-dodecahydro-2,4b-dimethylphenanthren-3-one, C19H28OS2

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Abstract. Epimer (3a): $M_r = 336.53$, orthorhombic, $P2_12_12_1$, $a = 8.096$ (2), $b = 3.338$ (3), $c = 26.465$ (4) Å, $V = 1786.5$ (8) Å^3, $Z = 4$, $D_x = 1.25$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 2.86$ cm^{-1}, $F(000) = 728$, $T = 290$ K. Final conventional $R = 0.028$ for 1962 unique observed reflections. Epimer (3b): $M_r = 336.53$, monoclinic, $P2_1/n$, $a = 11.340$ (3), $b = 6.386$ (3), $c = 25.159$ (6) Å, $\beta = 101.20$ (2)°, $V = 1787$ (1) Å^3, $Z = 4$, $D_x = 1.25$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 2.86$ cm^{-1}, $F(000) = 728$, $T = 290$ K. Final conventional $R = 0.043$ for 1121 unique observed reflections. The structure determinations confirm the chemically anticipated stereochemistry of the title compounds. Both epimers (key intermediates in the synthesis of a momilactone model) have a conformation with *trans-syn* coupled rings, in which the ring containing the dithiolane-ring substituted C atom has a chair conformation. Compound (3a) is shown to be the α-dithiolanyl epimer, compound (3b) the β-dithiolanyl epimer. The geometric features of the epimers are very similar.

Introduction. The fungitoxic momilactones (*e.g.* momilactone A, 1) form a class of rather unusual natural products, possessing a *trans-syn*-hydrophenanthrene skeleton (Kato, Aizawa, Tsunakawa, Sasaki, Kitahara & Takahashi, 1977; Tsunakawa, Ohba, Sasaki, Kabuto, Kato, Kitahara & Takahashi, 1976; Cartwright, Langcake, Pryce, Leworthy & Ride, 1981). An approach to their synthesis is in progress and has recently resulted (Sicherer-Roetman, Jansen & de Groot, 1984) in the synthesis of model compound (2), which possesses all the main features of the *BC* ring system of the momilactones. Key intermediates in this synthesis are the thiolanyl compounds (3a) and (3b) (Fig. 1), which were obtained *via* two different synthetic routes. It was clear from spectral evidence that both (3a) and (3b) possessed the desired *trans-syn*-fused ring system and that they were epimeric at the dithiolane-ring substituted C atom. However, the configuration at this C atom of each of the compounds, which is of vital importance for the synthesis of (2), could not be deduced from the spectra. Therefore the crystal structure of both compounds was determined to provide definite proof of their stereochemistry.

Experimental. Epimer (3a): crystals obtained by recrystallization from diisopropyl ether, unintentional selective crystallization of one optical isomer from racemic solution, plates, crystal 0.30 × 0.18 × 0.07 mm used. Enraf–Nonius CAD-4 diffractometer, Mo $K\alpha$ radiation, graphite-crystal monochromator.
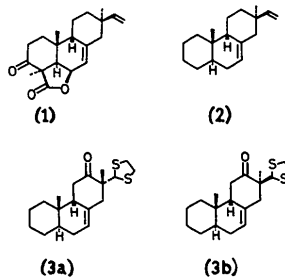

Fig. 1. Structural formulae of momilactone A (1), and model compounds (2, 3a, 3b).

Table 1. *Positional parameters and isotropic thermal parameters with e.s.d.'s (epimer 3a)*

U_{eq} as defined by Hamilton (1959).

	x	y	z	$U_{eq}/U(\text{Å}^2)$
S(1)	0·7060 (1)	−0·1356 (1)	0·8278 (1)	0·0433 (3)
S(2)	0·9556 (1)	0·1209 (1)	0·8378 (1)	0·0450 (3)
O(1)	0·7499 (4)	0·4478 (3)	0·7876 (1)	0·0627 (11)
C(1)	0·6768 (4)	0·3623 (4)	0·8170 (1)	0·0378 (10)
C(2)	0·6215 (5)	0·4287 (4)	0·8678 (1)	0·0401 (12)
C(3)	0·4332 (4)	0·4052 (4)	0·8735 (1)	0·0340 (11)
C(4)	0·3507 (4)	0·4752 (4)	0·9217 (1)	0·0357 (11)
C(5)	0·4273 (6)	0·6398 (5)	0·9351 (1)	0·0493 (13)
C(6)	0·3592 (6)	0·7083 (5)	0·9848 (2)	0·0586 (15)
C(7)	0·3857 (6)	0·5934 (5)	1·0283 (1)	0·0562 (15)
C(8)	0·3143 (5)	0·4283 (5)	1·0165 (1)	0·0496 (13)
C(9)	0·3773 (4)	0·3603 (4)	0·9660 (1)	0·0346 (10)
C(10)	0·3009 (5)	0·1946 (4)	0·9554 (1)	0·0455 (13)
C(11)	0·3440 (4)	0·1357 (4)	0·9035 (1)	0·0382 (11)
C(12)	0·3991 (4)	0·2274 (4)	0·8669 (1)	0·0299 (10)
C(13)	0·4472 (4)	0·1640 (4)	0·8157 (1)	0·0389 (11)
C(14)	0·6339 (4)	0·1892 (4)	0·8041 (1)	0·0316 (10)
C(15)	0·7346 (4)	0·0764 (4)	0·8392 (1)	0·0313 (10)
C(16)	0·9009 (5)	−0·1689 (5)	0·7965 (2)	0·0572 (15)
C(17)	1·0292 (5)	−0·0780 (5)	0·8249 (2)	0·0569 (15)
C(18)	0·6671 (5)	0·1538 (5)	0·7481 (1)	0·0456 (13)
C(19)	0·1666 (5)	0·4956 (5)	0·9094 (2)	0·0547 (15)
H(021)	0·651 (5)	0·549 (5)	0·868 (1)	0·060
H(022)	0·671 (5)	0·371 (5)	0·894 (1)	0·060
H(031)	0·389 (4)	0·458 (5)	0·846 (2)	0·060
H(051)	0·544 (5)	0·632 (5)	0·938 (1)	0·060
H(052)	0·409 (5)	0·711 (5)	0·908 (2)	0·060
H(061)	0·243 (5)	0·727 (5)	0·979 (2)	0·060
H(062)	0·413 (5)	0·812 (5)	0·988 (1)	0·060
H(071)	0·335 (5)	0·629 (5)	1·062 (1)	0·060
H(072)	0·510 (5)	0·582 (4)	1·031 (1)	0·060
H(081)	0·189 (5)	0·432 (4)	1·016 (1)	0·060
H(082)	0·340 (5)	0·344 (4)	1·045 (1)	0·060
H(091)	0·496 (5)	0·344 (4)	0·968 (1)	0·060
H(101)	0·184 (5)	0·205 (5)	0·956 (2)	0·060
H(102)	0·354 (4)	0·116 (5)	0·981 (1)	0·060
H(111)	0·335 (5)	0·022 (4)	0·898 (1)	0·060
H(131)	0·430 (5)	0·045 (5)	0·813 (1)	0·060
H(132)	0·389 (5)	0·223 (5)	0·794 (2)	0·060
H(151)	0·698 (5)	0·088 (4)	0·872 (1)	0·060
H(161)	0·887 (5)	−0·124 (5)	0·763 (1)	0·060
H(162)	0·908 (5)	−0·292 (5)	0·804 (1)	0·060
H(171)	1·126 (5)	−0·060 (5)	0·808 (1)	0·060
H(172)	1·042 (5)	−0·149 (5)	0·859 (1)	0·060
H(181)	0·785 (5)	0·161 (5)	0·741 (1)	0·060
H(182)	0·598 (5)	0·237 (5)	0·728 (1)	0·060
H(183)	0·631 (5)	0·036 (5)	0·739 (1)	0·060
H(191)	0·115 (5)	0·387 (5)	0·897 (1)	0·060
H(192)	0·156 (5)	0·581 (5)	0·885 (2)	0·060
H(193)	0·088 (5)	0·529 (5)	0·939 (2)	0·060

Table 2. *Positional parameters and isotropic thermal parameters with e.s.d.'s (epimer 3b)*

U_{eq} as defined by Hamilton (1959).

	x	y	z	$U_{eq}/U(\text{Å}^2)$
S(1)	−0·1210 (2)	−0·1953 (3)	0·0768 (1)	0·080 (1)
S(2)	0·0707 (2)	0·1171 (3)	0·1068 (1)	0·074 (1)
O(1)	0·2264 (4)	−0·1118 (7)	0·1986 (2)	0·063 (2)
C(1)	0·1367 (5)	−0·1303 (9)	0·2180 (2)	0·045 (3)
C(2)	0·1460 (5)	−0·120 (1)	0·2784 (3)	0·049 (3)
C(3)	0·0474 (5)	0·0153 (9)	0·2956 (2)	0·040 (2)
C(4)	0·0467 (5)	0·0216 (9)	0·3570 (2)	0·042 (3)
C(5)	0·1755 (6)	0·027 (1)	0·3901 (3)	0·064 (3)
C(6)	0·1807 (7)	0·006 (2)	0·4511 (3)	0·078 (4)
C(7)	0·1207 (8)	−0·192 (1)	0·4639 (3)	0·080 (4)
C(8)	−0·0068 (6)	−0·204 (1)	0·4332 (3)	0·063 (3)
C(9)	−0·0158 (5)	−0·175 (1)	0·3719 (2)	0·048 (4)
C(10)	−0·1459 (6)	−0·182 (1)	0·3425 (3)	0·065 (3)
C(11)	−0·1569 (6)	−0·138 (1)	0·2832 (3)	0·043 (3)
C(12)	−0·0707 (5)	−0·0506 (9)	0·2623 (2)	0·043 (3)
C(13)	−0·0792 (6)	−0·033 (1)	0·2022 (3)	0·048 (3)
C(14)	0·0151 (5)	−0·1734 (9)	0·1832 (2)	0·044 (3)
C(15)	0·0194 (5)	−0·143 (1)	0·1232 (3)	0·055 (3)
C(16)	−0·1552 (8)	0·050 (1)	0·0463 (4)	0·117 (5)
C(17)	−0·0647 (8)	0·214 (1)	0·0640 (4)	0·128 (5)
C(18)	−0·0162 (7)	−0·405 (1)	0·1916 (3)	0·061 (4)
C(19)	−0·0206 (8)	0·218 (1)	0·3680 (3)	0·070 (4)
H(021)	0·215 (5)	−0·066 (9)	0·294 (2)	0·06
H(022)	0·136 (5)	−0·27 (1)	0·292 (2)	0·06
H(031)	0·064 (5)	0·157 (9)	0·284 (2)	0·06
H(051)	0·221 (5)	−0·08 (1)	0·378 (2)	0·06
H(052)	0·205 (5)	0·160 (9)	0·381 (2)	0·06
H(061)	0·135 (5)	0·136 (9)	0·464 (2)	0·06
H(062)	0·260 (5)	0·018 (9)	0·471 (2)	0·06
H(071)	0·130 (4)	−0·216 (9)	0·508 (2)	0·06
H(072)	0·153 (6)	−0·30 (1)	0·454 (3)	0·06
H(081)	−0·052 (5)	−0·074 (9)	0·449 (2)	0·06
H(082)	−0·044 (5)	−0·34 (1)	0·440 (2)	0·06
H(091)	0·027 (5)	−0·305 (9)	0·359 (2)	0·06
H(101)	−0·189 (5)	−0·074 (9)	0·360 (2)	0·06
H(102)	−0·166 (5)	−0·31 (1)	0·344 (2)	0·06
H(111)	−0·233 (5)	−0·172 (9)	0·259 (2)	0·06
H(131)	−0·156 (5)	−0·084 (9)	0·182 (2)	0·06
H(132)	−0·072 (5)	0·11 (1)	0·192 (2)	0·06
H(151)	0·074 (5)	−0·22 (1)	0·117 (2)	0·06
H(181)	−0·003 (5)	−0·421 (9)	0·232 (2)	0·06
H(182)	0·043 (5)	−0·48 (1)	0·181 (2)	0·06
H(183)	−0·102 (5)	−0·426 (9)	0·166 (2)	0·06
H(191)	−0·087 (5)	0·25 (1)	0·342 (2)	0·06
H(192)	0·025 (5)	0·33 (1)	0·363 (2)	0·06
H(193)	−0·033 (5)	0·214 (9)	0·406 (2)	0·06

Lattice parameters from least-squares adjustment to setting angles of 25 general reflections with $22 < 2\theta < 41°$. Systematic absences $h00$, $h = 2n + 1$, $0k0$, $k = 2n + 1$, $00l$, $l = 2n + 1$. Intensity data of 9881 reflections (the full sphere with $2\theta < 46°$, $h \pm 8$, $k\ 0{\rightarrow}9$, $l\ 0{\rightarrow}28$), $\omega{-}2\theta$ scan technique, scan angle $0·85° + 0·347°$ tan θ, scan rate variable with a minimum of $2°$ min^{-1}. Two standard reflections monitored every 30 min, max. drift correction 1·026. Profile analysis (Lehmann & Larsen, 1974; Grant & Gabe, 1978). Empirical absorption correction, ψ scans (North, Phillips & Mathews, 1968, min. corr. 0·88, max. corr. 1·00; Walker & Stuart, 1983, min. corr. 0·75, max. corr. 1·26). Space-group symmetry-equivalent reflections averaged, $R_{int} = 0·024$, 2471 unique reflections, 1962 with $I > 3\sigma(I)$. Lorentz and polarization corrections. Solution by direct methods (*MULTAN*80, Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and *DIRDIF* (Beurskens, Bosman, Doesburg,

Van den Hark, Prick, Noordik, Beurskens, Gould & Parthasarathi, 1982). The highest two peaks of the two most probable *MULTAN* solutions were used as input to *DIRDIF* as two S atoms. The *DIRDIF* run based on the two S atoms from the second *MULTAN* solution gave all 22 non-H atoms as the top 22 peaks. Upon isotropic least-squares refinement (*SHELX*76, Sheldrick, 1976), convergence was achieved at $R = 0·081$. H atoms located from a difference Fourier map. Additional refinement with all non-H atoms treated anisotropically and fixed thermal parameters for H atoms ($U = 0·006$ Å^2) converged at $R = 0·028$, $wR = 0·033$ for the 1962 observed reflections and 283 variables. $\sum w(|F_o| - |F_c|)^2$ minimized with $w = 1/[\sigma^2(F_o) + 0·00015\ F_o^2]$ with $\sigma^2(F_o)$ from counting statistics. $(\Delta/\sigma)_{max}$ in last least-squares cycle (full-matrix) $< 0·10$. Final $\Delta\rho$ excursions $< 0·22$ e Å^{-3}. Atomic form factors from *SHELX*76. Absolute configuration from comparison of observed and calculated Bijvoet differences $\Delta F_o = F_o(h) - F_o(-h)$, $\Delta F_c = F_c(h) - F_c(-h)$; Bijvoet coefficient $B = \sum(\Delta F_c . \Delta F_o)/$

Table 3. Bond lengths (Å) with e.s.d.'s in parentheses

For each atom the top line refers to (3a), the bottom line to (3b).

S(1)–C(15)	1·808 (3)	C(1)–C(2)	1·522 (4)	C(4)–C(5)	1·547 (4)	C(7)–C(8)	1·525 (6)	C(12)–C(13)	1·504 (4)
	1·813 (7)		1·503 (8)		1·535 (8)		1·503 (10)		1·501 (8)
S(1)–C(16)	1·802 (4)	C(1)–C(14)	1·523 (4)	C(4)–C(9)	1·530 (4)	C(8)–C(9)	1·540 (4)	C(13)–C(14)	1·556 (4)
	1·757 (8)		1·509 (7)		1·525 (8)		1·537 (9)		1·542 (8)
S(2)–C(15)	1·828 (3)	C(2)–C(3)	1·545 (4)	C(4)–C(19)	1·535 (4)	C(9)–C(10)	1·539 (4)	C(14)–C(15)	1·553 (4)
	1·832 (6)		1·542 (8)		1·524 (9)		1·517 (9)		1·531 (8)
S(2)–C(17)	1·795 (4)	C(3)–C(4)	1·553 (4)	C(5)–C(6)	1·535 (4)	C(10)–C(11)	1·501 (4)	C(14)–C(18)	1·535 (4)
	1·804 (8)		1·547 (8)		1·531 (10)		1·498 (10)		1·542 (9)
O(1)–C(1)	1·209 (4)	C(3)–C(12)	1·518 (4)	C(6)–C(7)	1·513 (6)	C(11)–C(12)	1·313 (4)	C(16)–C(17)	1·489 (6)
	1·217 (6)		1·496 (8)		1·497 (12)		1·321 (8)		1·472 (5)

$\sum |\Delta F_c.\Delta F_o|$ (Beurskens, Noordik & Beurskens, 1980) where the sum is over the most significant Bijvoet pairs selected according to $|\Delta F_o| > N1.\sigma(\Delta F_o)$ and $|\Delta F_c| > N2[F_c(h)-F_c(-h)]/2$; $B = 0.45$ (14) for 11 selected pairs with $N1 = 2$, $N2 = 0.02$ (Mo radiation!) strongly indicating that the parameter set given in Table 1 gives the absolute configuration.

Epimer (3b): crystals obtained by recrystallization from hexane, needles, crystal $0.37 \times 0.10 \times 0.10$ mm used. Enraf–Nonius CAD-4 diffractometer, Mo $K\alpha$ radiation, graphite-crystal monochromator. Lattice parameters from least-squares adjustment to setting angles of 22 general reflections with $13 < 2\theta < 31°$. Systematic absences $h0l$, $h + l = 2n + 1$, $0k0$, $k = 2n + 1$. Intensity data of 6664 reflections (the full sphere with $2\theta < 40°$, $h \pm 10$, $k\,0\to6$, $l\,0\to24$), ω–2θ scan technique, scan angle 1°, scan rate variable with a minimum of 2° min^{-1}. Three standard reflections monitored every 30 min, max. drift correction 1·023. Profile analysis (Lehmann & Larsen, 1974; Grant & Gabe, 1978). Empirical absorption correction, ψ scans (North, Phillips & Mathews, 1968, min. corr. 0·91, max. corr. 1·00; Walker & Stuart, 1983, min. corr. 0·78, max. corr. 1·14). Laue symmetry-equivalent reflections averaged, $R_{int} = 0.019$, 1618 unique reflections, 1121 with $I > 3\sigma(I)$. Lorentz and polarization corrections. Solution by direct methods (*MULTAN*80, Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Upon isotropic least-squares refinement (*SHELX*76, Sheldrick, 1976), convergence was achieved at $R = 0.114$. H atoms located from difference Fourier map except at C(16) and C(17); these two C atoms show some disorder (see thermal parameters in Table 1). Additional refinement with all non-H atoms treated anisotropically and fixed thermal parameters for H atoms ($U = 0.06$ Å^2), omitting those at C(16) and C(17), converged at $R = 0.043$, $wR = 0.051$ for the 1121 observed reflections and 272 variables. $\sum w(|F_o| - |F_c|)^2$ minimized with $w = 1/[\sigma^2(F_o) + 0.0002\,F_o^2]$ with $\sigma^2(F_o)$ from counting statistics. $(\Delta/\sigma)_{max}$ in last refinement cycle (full-matrix) < 0.2. Final $\Delta\rho$ excursions < 0.26 e Å^{-3}. Atomic form factors from *SHELX*76.

Discussion. Final positional and isotropic thermal parameters are given in Table 1 (epimer 3a) and Table

Table 4. Bond angles (°) with e.s.d.'s in parentheses

	Epimer (3a)	Epimer (3b)
C(15)–S(1)–C(16)	96·6 (1)	102·0 (4)
C(15)–S(2)–C(17)	98·1 (1)	100·1 (4)
O(1)–C(1)–C(2)	119·8 (3)	120·2 (5)
O(1)–C(1)–C(14)	121·8 (3)	121·7 (5)
C(2)–C(1)–C(14)	118·4 (3)	118·1 (5)
C(1)–C(2)–C(3)	109·3 (3)	113·3 (5)
C(2)–C(3)–C(4)	117·2 (3)	116·1 (5)
C(2)–C(3)–C(12)	107·0 (3)	107·6 (5)
C(4)–C(3)–C(12)	112·6 (3)	112·9 (5)
C(3)–C(4)–C(5)	110·5 (3)	110·7 (5)
C(3)–C(4)–C(9)	109·5 (3)	108·4 (5)
C(5)–C(4)–C(9)	108·8 (3)	108·9 (5)
C(3)–C(4)–C(19)	106·6 (3)	107·6 (5)
C(5)–C(4)–C(19)	109·9 (3)	110·0 (6)
C(9)–C(4)–C(19)	111·6 (3)	111·3 (5)
C(4)–C(5)–C(6)	112·5 (3)	112·9 (6)
C(5)–C(6)–C(7)	111·4 (3)	111·0 (7)
C(6)–C(7)–C(8)	111·3 (3)	111·4 (7)
C(7)–C(8)–C(9)	112·6 (3)	112·3 (6)
C(4)–C(9)–C(8)	112·9 (3)	113·5 (5)
C(4)–C(9)–C(10)	111·5 (3)	111·0 (5)
C(8)–C(9)–C(10)	110·8 (3)	110·8 (5)
C(9)–C(10)–C(11)	111·5 (3)	111·4 (6)
C(10)–C(11)–C(12)	124·4 (3)	123·4 (6)
C(3)–C(12)–C(11)	123·0 (3)	123·1 (6)
C(3)–C(12)–C(13)	113·6 (3)	114·8 (5)
C(11)–C(12)–C(13)	123·2 (3)	121·8 (6)
C(12)–C(13)–C(14)	112·4 (3)	110·8 (5)
C(1)–C(14)–C(13)	107·8 (3)	108·9 (5)
C(1)–C(14)–C(15)	108·7 (1)	110·4 (5)
C(13)–C(14)–C(15)	108·1 (1)	112·8 (5)
C(1)–C(14)–C(18)	111·0 (3)	107·7 (5)
C(13)–C(14)–C(18)	109·6 (3)	108·9 (5)
C(15)–C(14)–C(18)	111·7 (3)	108·0 (5)
S(1)–C(15)–S(2)	108·7 (1)	107·5 (3)
S(1)–C(15)–C(14)	115·2 (1)	114·7 (4)
S(2)–C(15)–C(14)	112·3 (1)	114·3 (4)
S(1)–C(16)–C(17)	107·5 (3)	114·9 (6)
S(2)–C(17)–C(16)	109·6 (3)	113·5 (6)

2 (epimer 3b).* Molecular-geometry data are collected in Tables 3 and 4. The crystallographic atomic-numbering scheme is given in Fig. 2. A stereoscopic view of both epimers, showing the molecular conformation, is given in Fig. 3.

The geometric features of epimers (3a) and (3b) are, apart from the difference in stereochemistry at C(14), very similar. Bond distances, bond angles and torsion angles agree without significant differences, except for the geometry of the dithiolane ring where a comparison is impossible because of the slight disorder at C(16) and
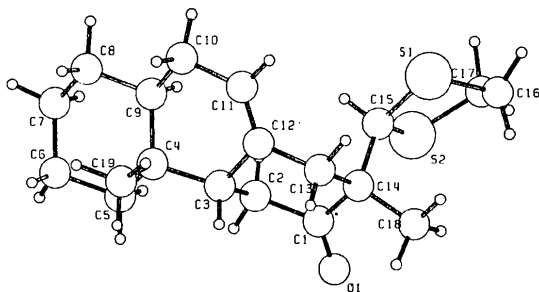
Fig. 2. Crystallographic atomic-numbering scheme. [Epimer (3a) in minimum-overlap view.]
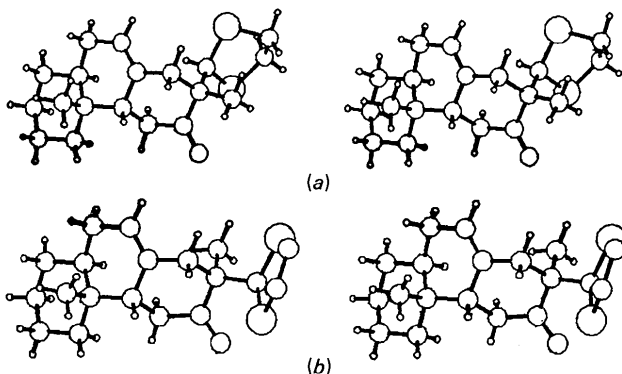

(a)

(b)

Fig. 3. Stereoview of the molecules showing the stereochemistry at C(14). (a) Epimer (3a), (b) epimer (3b); identical view directions.

C(17). The stereochemical difference of the epimers, which is clearly shown in Fig. 3, is also expressed by the values of the torsion angles involving the atoms C(15) and C(18). Some selected values are: O(1)—C(1)—C(14)—C(18) (3a) −10·0 (5), (3b) 105·8 (5)°; C(2)—C(1)—C(14)—C(15) (3a) −68·5 (5), (3b) 170·9 (5)°;

O(1)—C(1)—C(14)—C(15)   (3a)   113·1 (5),   (3b) −11·9 (5)°; C(2)—C(1)—C(14)—C(18) (3a) 168·4 (5), (3b) −71·4 (5)°; C(12)—C(13)—C(14)—C(15) (3a) 69·5 (5), (3b) −173·7 (5)°; C(12)—C(13)—C(14)—C(18) (3a) −168·6 (5), (3b) 66·4 (5)°.

The H atoms in both structures are well determined and refined C—H bond distances are between 0·86 and 1·11 Å.

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Struktur des Radikaldimeren N-tert-Butyl-N-{(5-tert-butyl-1,3,7,8-tetraphenyl-2,4,9-trioxa-5-azatricyclo[4.2.1.0³·⁷]non-8-yl)methylen}amin-N-oxid, $C_{38}H_{40}N_2O_4$, bei 210 K

Von Hans Günter Aurich, Gerhard Baum, Werner Massa* und Klaus-Dieter Mogendorf

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Abstract. $M_r = 588·75$, monoclinic, $P2_1/c$, $a = 10·566$ (4), $b = 15·629$ (3), $c = 38·579$ (8) Å, $\beta = 90·34$ (2)°, $V = 6375$ (3) Å³, $Z = 8$, $D_x = 1·227\ \mathrm{g\,cm^{-3}}$, Mo $K\alpha$, $\lambda = 0·7107$ Å, $\mu = 0·74\ \mathrm{cm^{-1}}$, $F(000) = 2512$, $T = 210$ K, $R = 0·055$ for 5608 reflections. There are two independent molecules in the asymmetric unit, differing mainly by the torsion of a phenyl substituent at an angle of about 16°. The

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