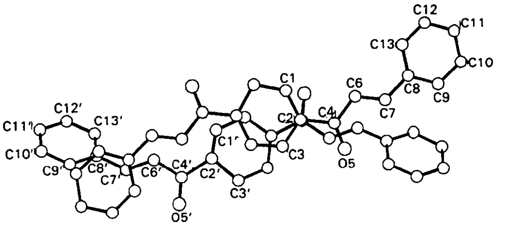

Fig. 1. The intermolecular overlapping of reactive molecules, viewed along the normal to the central benzene ring.

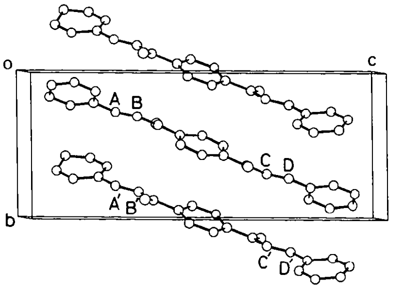

Fig. 2. The crystal structure projected onto the (100) plane. Intermolecular distances *A–A'*, *B–B'*, *C–C'*, and *D–D'* are 3·973, 4·086, 3·903, and 3·955 Å, respectively.

Consequently, it is noteworthy that 1,4-DCB anomalously dupledimerizes in spite of a non-parallel arrangement of both photoreactive C—C double-bond pairs. Although the solid-state photodimerization of 7-methoxycoumarin, packed non-parallel in crystals, has been reported (Ramasubbu, Row, Venkatesan, Ramamurthy & Rao, 1982), this reaction is the first example of a non-parallel diolefinic compound to dupledimerize on irradiation.

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5-Benzylidene-1,2,3,4,4a,5,6,7,8,9a-decahydro-4a-morpholino-9-phenylxanthene, $C_{30}H_{35}NO_2$ (DBM), and 5-Benzylidene-1,2,3,4,4a,5,6,7,8,9a-decahydro-9-phenyl-4a-piperidinoxanthene, $C_{31}H_{37}NO$ (DBP)

By M. N. Ponnuswamy and James Trotter

Department of Chemistry, The University of British Columbia, Vancouver, BC, Canada V6T 1Y6

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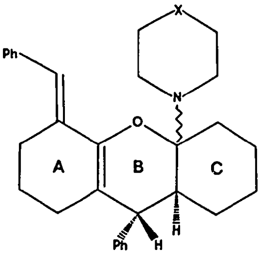
Abstract. DBM, DBP, $M_r = 441{\cdot}62$, 439·65, triclinic, $P\bar{1}$, $a = 10{\cdot}945\ (2)$, 10·879 (2), $b = 13{\cdot}545\ (3)$, 13·502 (5), $c = 9{\cdot}478\ (1)$, 9·587 (2) Å, $\alpha = 99{\cdot}62\ (2)$, 99·12 (2), $\beta = 114{\cdot}36\ (1)$, 114·55 (2), $\gamma = 73{\cdot}02\ (2)$, 73·66 (2)°, $V = 1222{\cdot}4\ (4)$, 1227·8 (7) Å^3, $Z = 2$, D_m(flotation) = 1·160, 1·185, $D_x = 1{\cdot}199$, 1·189 g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 0{\cdot}748$, 0·690 cm^{-1}, $F(000) = 476$, 476, room temperature, final $R = 0{\cdot}059$, 0·051 for 2579, 3022 reflections. The crystals are isostructural, both molecules having *cis*-fused *B*/*C* rings, with the morpholino and piperidino substituents axially oriented with respect to the *C* ring.

Introduction. In a study of the synthesis of dihydropyrans (Balaji Rao & Bhide, 1969; Reddy, 1982; Reddy & Balaji Rao, 1982), spectroscopic data, namely IR and NMR, suggested two different configurations for (1) and (2), with *trans*- and *cis*-fused *B*/*C* ring junctions, respectively. Since it is unusual that a remote oxygen atom should play such a decisive role in the course of the reaction, crystal structure studies have been undertaken to establish the molecular configurations conclusively.



(1) DBM X = O
(2) DBP X = CH_2

0108-2701/84/030511-04$01.50

Experimental. In the following text, the quantities in square brackets refer to the DBP compound. Parameters after which no brackets follow are the same for both title compounds.

Colorless crystals (from benzene), 0·25 × 0·05 × 0·15 mm [0·2 × 0·15 × 0·3 mm], CAD-4 diffractometer, graphite-monochromatized Mo *K*α radiation, $\theta \le 27{\cdot}5°$, ω–2θ scan, ω-scan width (0·70 +

Table 1. *Final positional (fractional* ×10⁴, H ×10³) *and isotropic thermal parameters* (Å² ×10³) *with e.s.d.'s in parentheses*

$$U_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	(i) DBM				(ii) DBP			
	x	y	z	$U_{\rm eq}/U_{\rm iso}$	x	y	z	$U_{\rm eq}/U_{\rm iso}$
C(1)	2717 (6)	4053 (4)	7551 (6)	54	2806 (3)	4057 (2)	7579 (3)	44
C(2)	4220 (7)	3674 (5)	7702 (8)	71	4324 (3)	3684 (3)	7756 (4)	57
C(3)	5176 (6)	3202 (5)	9229 (7)	64	5255 (3)	3218 (2)	9284 (4)	57
C(4)	4658 (5)	2393 (4)	9614 (6)	48	4708 (2)	2405 (2)	9658 (3)	41
C(4a)	3177 (4)	2853 (3)	9571 (5)	35	3218 (2)	2857 (1)	9568 (2)	30
C(5)	2268 (5)	399 (3)	9458 (5)	38	2272 (2)	393 (2)	9431 (2)	34
C(5a)	2333 (4)	1292 (3)	8807 (5)	37	2360 (2)	1289 (2)	8801 (2)	33
C(6)	1753 (6)	−431 (4)	8265 (6)	47	1760 (3)	−434 (2)	8259 (3)	44
C(7)	2268 (6)	−559 (3)	6967 (6)	51	2299 (3)	−553 (2)	6981 (3)	49
C(8)	1774 (6)	454 (4)	6167 (6)	49	1833 (3)	453 (2)	6188 (3)	46
C(8a)	2065 (4)	1353 (3)	7319 (5)	35	2118 (2)	1351 (2)	7325 (2)	32
C(9)	2136 (5)	2298 (3)	6729 (5)	38	2224 (2)	2298 (2)	6757 (2)	32
C(9a)	2219 (5)	3224 (3)	7932 (5)	36	2291 (2)	3218 (2)	7941 (2)	31
C(10)	2690 (5)	345 (3)	10990 (5)	45	2689 (3)	344 (2)	10945 (3)	40
C(11)	2711 (5)	−469 (3)	11858 (5)	43	2688 (3)	−468 (2)	11816 (3)	40
C(12)	3803 (6)	−725 (4)	13266 (6)	56	3776 (3)	−704 (2)	13235 (3)	50
C(13)	3866 (7)	−1485 (4)	14126 (6)	65	3830 (3)	−1450 (2)	14113 (3)	61
C(14)	2820 (7)	−1994 (4)	13597 (7)	64	2763 (3)	−1968 (2)	13578 (4)	61
C(15)	1719 (6)	−1742 (4)	12220 (7)	60	1691 (3)	−1740 (2)	12208 (4)	59
C(16)	1650 (6)	−990 (4)	11344 (6)	51	1633 (3)	−997 (2)	11307 (3)	48
C(17)	975 (5)	2589 (3)	5161 (5)	39	1083 (2)	2579 (2)	5193 (2)	34
C(18)	−390 (5)	3005 (4)	5001 (7)	54	−313 (3)	2978 (2)	4980 (3)	47
C(19)	−1430 (6)	3242 (5)	3547 (8)	67	−1330 (3)	3215 (2)	3551 (3)	57
C(20)	−1111 (8)	3068 (5)	2258 (7)	76	−996 (3)	3046 (2)	2273 (3)	60
C(21)	228 (8)	2646 (5)	2391 (7)	75	384 (3)	2630 (2)	2451 (3)	60
C(22)	1251 (6)	2420 (4)	3830 (6)	56	1399 (3)	2407 (2)	3886 (3)	50
C(23)	1849 (6)	4360 (5)	10675 (7)	62	1852 (2)	4357 (2)	10603 (3)	39
C(24)	2099 (8)	5254 (5)	11883 (9)	84	2031 (3)	5267 (2)	11766 (3)	51
C(25)					2779 (3)	4912 (2)	13393 (3)	56
C(26)	4145 (7)	4236 (5)	13513 (7)	66	4150 (3)	4160 (2)	13539 (3)	45
C(27)	3969 (7)	3326 (4)	12356 (6)	57	3934 (3)	3288 (2)	12318 (3)	42
N	3189 (4)	3681 (3)	10773 (4)	39	3212 (2)	3674 (1)	10762 (2)	31
O(1)	2679 (3)	2076 (2)	9921 (3)	45	2697 (2)	2068 (1)	9892 (2)	39
O(2)	2869 (5)	4918 (4)	13421 (5)	87				
H1(C1)	258 (4)	470 (4)	822 (5)	54 (14)	275 (2)	469 (2)	832 (3)	53 (7)
H2(C1)	207 (5)	431 (3)	648 (5)	51 (13)	227 (2)	427 (2)	654 (3)	41 (6)
H1(C2)	451 (6)	424 (4)	755 (6)	83 (18)	461 (3)	431 (2)	772 (3)	70 (8)
H2(C2)	427 (5)	316 (4)	678 (6)	79 (18)	438 (3)	315 (2)	689 (3)	54 (7)
H1(C3)	531 (4)	375 (3)	1008 (5)	49 (13)	534 (3)	379 (2)	1010 (3)	54 (7)
H2(C3)	605 (6)	289 (4)	917 (6)	77 (18)	619 (3)	290 (2)	936 (3)	71 (8)
H1(C4)	464 (4)	176 (3)	882 (5)	39 (11)	465 (2)	184 (2)	889 (2)	34 (6)
H2(C4)	523 (4)	210 (3)	1062 (5)	40 (12)	531 (2)	213 (2)	1071 (3)	43 (6)
H1(C6)	206 (4)	−104 (3)	872 (4)	35 (12)	211 (2)	−112 (2)	879 (2)	39 (6)
H2(C6)	65 (5)	−23 (3)	777 (5)	62 (15)	73 (3)	−24 (2)	777 (3)	56 (7)
H1(C7)	197 (4)	−113 (3)	621 (5)	56 (14)	197 (3)	−108 (2)	623 (3)	62 (8)
H2(C7)	338 (5)	−75 (3)	742 (5)	49 (13)	341 (3)	−79 (2)	750 (3)	57 (7)
H1(C8)	219 (5)	42 (3)	542 (5)	57 (15)	232 (3)	42 (2)	544 (4)	84 (10)
H2(C8)	77 (6)	58 (4)	548 (6)	76 (18)	86 (3)	58 (2)	546 (3)	62 (8)
H(C9)	298 (4)	209 (3)	652 (4)	35 (11)	317 (2)	205 (2)	659 (2)	45 (6)
H(C9a)	128 (4)	352 (3)	792 (4)	31 (11)	135 (2)	350 (2)	788 (2)	30 (5)
H(C10)	302 (4)	89 (3)	1160 (5)	45 (12)	311 (2)	88 (2)	1164 (3)	43 (6)
H(C12)	454 (5)	−36 (4)	1368 (6)	76 (18)	454 (3)	−33 (2)	1365 (3)	63 (8)
H(C13)	462 (5)	−165 (3)	1510 (5)	56 (15)	462 (3)	−160 (2)	1523 (3)	62 (8)
H(C14)	290 (4)	−252 (3)	1414 (5)	46 (13)	289 (3)	−248 (2)	1428 (3)	75 (9)
H(C15)	98 (6)	−211 (4)	1182 (6)	83 (19)	89 (4)	−209 (3)	1175 (4)	95 (11)
H(C16)	81 (5)	−83 (3)	1035 (5)	57 (14)	84 (3)	−81 (2)	1036 (3)	54 (8)
H(C18)	−58 (5)	308 (4)	587 (5)	54 (15)	−58 (3)	312 (2)	592 (3)	70 (8)
H(C19)	−230 (6)	352 (4)	362 (6)	69 (18)	−233 (4)	356 (3)	340 (4)	108 (12)
H(C20)	−181 (5)	324 (4)	128 (6)	69 (16)	−170 (3)	321 (2)	124 (3)	56 (7)
H(C21)	44 (6)	254 (5)	141 (7)	110 (23)	56 (3)	250 (2)	146 (4)	89 (10)
H(C22)	219 (6)	210 (4)	394 (6)	86 (20)	250 (4)	204 (3)	409 (3)	90 (10)
H1(C23)	124 (5)	464 (4)	962 (6)	60 (15)	139 (2)	462 (2)	957 (3)	38 (6)
H2(C23)	134 (5)	395 (4)	1091 (6)	72 (17)	125 (3)	395 (2)	1075 (3)	51 (7)
H1(C24)	117 (6)	577 (4)	1182 (6)	85 (18)	113 (3)	578 (2)	1158 (3)	59 (7)
H2(C24)	254 (7)	567 (5)	1162 (7)	104 (26)	272 (3)	563 (2)	1162 (3)	79 (9)
H1(C25)					226 (4)	455 (3)	1369 (4)	105 (12)
H2(C25)					298 (3)	550 (2)	1419 (3)	62 (8)
H1(C26)	472 (5)	462 (4)	1331 (6)	71 (17)	476 (3)	455 (2)	1343 (3)	71 (9)
H2(C26)	467 (6)	397 (4)	1461 (7)	80 (18)	462 (2)	388 (2)	1456 (3)	47 (7)
H1(C27)	353 (6)	289 (4)	1257 (6)	80 (19)	352 (3)	288 (2)	1253 (3)	72 (9)
H2(C27)	490 (6)	283 (5)	1245 (7)	98 (22)	492 (3)	280 (2)	1245 (3)	50 (7)

$0{\cdot}35\tan\theta)^\circ$ $[(1{\cdot}10 + 0{\cdot}35\tan\theta)^\circ]$ extended 25% on each side for background measurement; cell parameters by least-squares fit to observed $\sin^2\theta$ values for 17 centered reflections with $12 < \theta < 18^\circ$, intensity and orientation controls regularly, $< \pm 1\%$ deviation throughout data collection; 5555 [5567] independent reflections, 2579 [3022] with $I \geq 1{\cdot}5[2]\sigma(I)$, where $\sigma^2(I) = S + 2B + [0{\cdot}04(S - B)]^2$, S = total peak count and B = time-averaged background; Lp corrections (no absorption correction); structures solved by *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), refined (on F) by full-matrix least squares; H atoms from a difference synthesis, isotropic; final $R = 0{\cdot}059$ [0·051], $R_w = 0{\cdot}062$ [0·058], 438 [446] variables; $R = 0{\cdot}155$ [0·108], $R_w = 0{\cdot}062$ [0·058] for all data; unit weights $[w = 1/\sigma^2(F)]$; $(\Delta/\sigma)_{\rm mean}$ and $(\Delta/\sigma)_{\rm max}$ 0·012 [0·005] and 0·121 [0·027] respectively; $S = 0{\cdot}869$ [2·040]; random fluctuations of $\pm 0{\cdot}14$ e Å^{-3} [0·35 e Å^{-3}] on final difference map; scattering factors from Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965); local adaptations of standard computer programs, *ORFLS* (Busing, Martin & Levy, 1962), *ORFFE* (Busing, Martin & Levy, 1964), and *ORTEP*II (Johnson, 1976).

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

	DBM	DBP		DBM	DBP
C(1)–C(2)	1·526 (8)	1·528 (4)	C(11)–C(12)	1·388 (7)	1·393 (3)
C(1)–C(9a)	1·531 (6)	1·536 (3)	C(11)–C(16)	1·408 (7)	1·397 (3)
C(2)–C(3)	1·506 (9)	1·506 (4)	C(12)–C(13)	1·386 (7)	1·386 (4)
C(3)–C(4)	1·525 (7)	1·536 (4)	C(13)–C(14)	1·382 (8)	1·396 (4)
C(4)–C(4a)	1·543 (6)	1·534 (3)	C(14)–C(15)	1·373 (8)	1·354 (4)
C(4a)–C(9a)	1·541 (6)	1·531 (3)	C(15)–C(16)	1·384 (7)	1·396 (4)
C(4a)–N	1·457 (5)	1·459 (3)	C(17)–C(18)	1·387 (7)	1·398 (3)
C(4a)–O(1)	1·455 (5)	1·464 (2)	C(17)–C(22)	1·383 (6)	1·401 (3)
C(5)–C(5a)	1·478 (6)	1·477 (3)	C(18)–C(19)	1·392 (7)	1·373 (4)
C(5)–C(6)	1·510 (6)	1·501 (3)	C(19)–C(20)	1·370 (9)	1·386 (4)
C(5)–C(10)	1·338 (6)	1·336 (3)	C(20)–C(21)	1·369 (9)	1·393 (4)
C(5a)–C(8a)	1·329 (6)	1·339 (3)	C(21)–C(22)	1·374 (8)	1·373 (4)
C(5a)–O(1)	1·384 (5)	1·373 (2)	C(23)–C(24)	1·525 (8)	1·520 (3)
C(6)–C(7)	1·518 (7)	1·535 (3)	C(23)–N	1·461 (6)	1·466 (3)
C(7)–C(8)	1·525 (6)	1·516 (3)	C(24)–O(2)	1·424 (9)	
C(8)–C(8a)	1·507 (6)	1·505 (3)	C(24)–C(25)		1·512 (4)
C(8a)–C(9)	1·513 (6)	1·517 (3)	C(26)–O(2)	1·409 (7)	
C(9)–C(9a)	1·545 (6)	1·540 (3)	C(25)–C(26)		1·515 (4)
C(9)–C(17)	1·524 (6)	1·517 (3)	C(26)–C(27)	1·507 (7)	1·517 (3)
C(10)–C(11)	1·472 (6)	1·480 (3)	C(27)–N	1·469 (6)	1·469 (3)

Discussion. Final atomic parameters are in Table 1,* bond lengths and angles in Tables 2 and 3.

The crystals are isostructural, and both molecules have a similar configuration with a *cis*-fused *B*/*C* junction in the xanthene ring system (Fig. 1); the spectroscopic data therefore require reinterpretation.

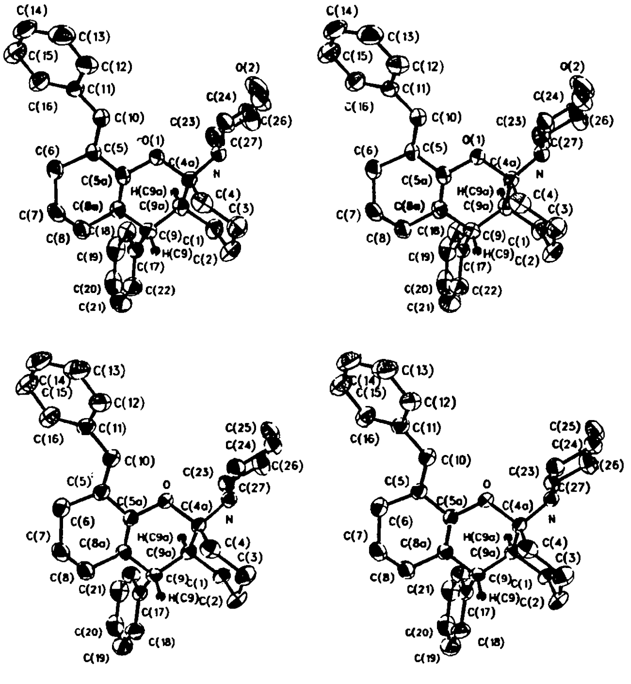


Fig. 1. Stereograms of DBM (top) and DBP (bottom). Thermal ellipsoids are at 50% probability.

Table 3. *Bond angles* (°) *with e.s.d.'s in parentheses*

	DBM	DBP		DBM	DBP		DBM	DBP
C(2)–C(1)–C(9a)	112·2 (4)	112·1 (2)	C(5a)–C(8a)–C(8)	121·3 (4)	121·3 (2)	C(9)–C(17)–C(22)	120·5 (4)	120·2 (2)
C(1)–C(2)–C(3)	112·8 (5)	111·9 (2)	C(5a)–C(8a)–C(9)	121·5 (4)	121·3 (2)	C(18)–C(17)–C(22)	117·4 (5)	117·4 (2)
C(2)–C(3)–C(4)	112·9 (5)	113·1 (2)	C(8)–C(8a)–C(9)	117·1 (4)	117·3 (2)	C(17)–C(18)–C(19)	120·6 (6)	121·3 (3)
C(3)–C(4)–C(4a)	110·5 (4)	110·7 (2)	C(8a)–C(9)–C(9a)	112·5 (4)	112·3 (2)	C(18)–C(19)–C(20)	120·1 (6)	120·4 (3)
C(4)–C(4a)–C(9a)	108·6 (4)	108·4 (2)	C(8a)–C(9)–C(17)	112·4 (4)	111·7 (2)	C(19)–C(20)–C(21)	120·1 (6)	119·4 (3)
C(4)–C(4a)–N	109·6 (4)	109·8 (2)	C(9a)–C(9)–C(17)	111·9 (4)	112·4 (2)	C(20)–C(21)–C(22)	119·4 (6)	119·9 (3)
C(4)–C(4a)–O(1)	110·4 (3)	110·1 (2)	C(1)–C(9a)–C(4a)	110·0 (4)	110·1 (2)	C(17)–C(22)–C(21)	122·3 (6)	121·6 (3)
C(9a)–C(4a)–N	112·7 (3)	113·6 (2)	C(1)–C(9a)–C(9)	112·2 (4)	111·9 (2)	C(24)–C(23)–N	108·5 (5)	110·4 (2)
C(9a)–C(4a)–O(1)	109·2 (3)	109·1 (2)	C(4a)–C(9a)–C(9)	110·3 (3)	110·8 (2)	C(23)–C(24)–O(2)	112·7 (6)	
N–C(4a)–O(1)	106·5 (3)	105·8 (2)	C(5)–C(10)–C(11)	129·2 (4)	129·2 (2)	C(27)–C(26)–O(2)	112·5 (5)	
C(5a)–C(5)–C(6)	114·4 (4)	114·9 (2)	C(10)–C(11)–C(12)	119·2 (5)	118·6 (2)	C(23)–C(24)–C(25)		111·5 (2)
C(5a)–C(5)–C(10)	120·9 (4)	120·1 (2)	C(10)–C(11)–C(16)	122·9 (4)	123·4 (2)	C(24)–C(25)–C(26)		108·7 (2)
C(6)–C(5)–C(10)	124·6 (4)	124·9 (2)	C(12)–C(11)–C(16)	117·9 (4)	117·9 (2)	C(25)–C(26)–C(27)		111·2 (2)
C(5)–C(5a)–C(8a)	124·3 (4)	124·2 (2)	C(11) C(12)–C(13)	121·3 (6)	121·5 (3)	C(26)–C(27)–N	110·4 (5)	112·0 (2)
C(5)–C(5a)–O(1)	112·3 (3)	112·6 (2)	C(12)–C(13)–C(14)	120·0 (6)	119·5 (3)	C(4a)–N–C(23)	116·8 (4)	116·5 (2)
C(8a)–C(5a)–O(1)	123·4 (4)	123·2 (2)	C(13)–C(14)–C(15)	119·7 (5)	119·7 (3)	C(4a)–N–C(27)	113·7 (3)	113·0 (2)
C(5)–C(6)–C(7)	111·1 (4)	110·7 (2)	C(14)–C(15)–C(16)	120·8 (6)	121·3 (3)	C(23)–N–C(27)	108·9 (4)	109·3 (2)
C(6)–C(7)–C(8)	110·4 (4)	111·0 (2)	C(11)–C(16)–C(15)	120·3 (5)	120·1 (3)	C(4a)–O(1)–C(5a)	118·1 (3)	118·4 (2)
C(7)–C(8)–C(8a)	111·8 (4)	111·8 (2)	C(9)–C(17)–C(18)	122·0 (4)	122·3 (2)	C(24)–O(2)–C(26)	109·6 (5)	

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[*] Lists of structure factors, anisotropic thermal parameters, bond distances and angles involving hydrogen atoms, torsion angles and the packing diagrams have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38982 (53 pp.). Copies may be obtained through the Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The detailed conformations and dimensions are also closely similar in the two structures. Rings *A* and *B* have half-chair conformations (Table 4), with approximately planar central C(5a)=C(8a) double-bond systems and the outer atoms displaced above and below the planes by about ±0·048 (5) Å [±0·044 (3) Å]. The *C* rings have chair conformations (Table 4), with torsion angles in the range ±50·2 (7) – ±60·3 (5)° [±50·1 (3) – ±60·7 (2)°]. The morpholino [piperidino] ring, C(9)-phenyl substituent, and C(9a) hydrogen atom are all on the same side of the rough plane of the xanthene nucleus, with the C(9) hydrogen atom on the opposite side [so that H(C9) and H(C9a) are *trans*-diaxial with respect to the *B* ring]. The morpholino and piperidino rings have chair conformations (Table 4), torsion angles ±56·2 (7) – ±58·9 (8)° [±53·5 (3) – ±59·7 (3)°], and the C(5)=C(10) double-bond system and the phenyl groups are essentially planar. The C(9)-phenyl substituent ring plane is approximately normal to the *B* ring, and the C(10)-phenyl substituent is rotated 39·4 (1)° [38·7 (1)°] out of the plane of the C(5)=C(10) benzylidene bond.

Bond distances and angles in the two molecules (Tables 2 and 3) are closely similar, apart from those in the morpholino [*vs* the piperidino] ring, and are close to expected values. In the xanthene nucleii the two C—O bond lengths differ significantly, C(sp^2)—O = 1·384 (5) [1·373 (2)] and C(sp^3)—O = 1·455 (5) [1·464 (2)] Å, as found in related structures (Andreetti, Bocelli & Sgarabotto, 1974; Howard, Johnstone, King & Lessinger, 1976). C=C bonds are in the range 1·329 (6)–1·339 (3) Å, with other C—C bonds within the ranges expected for the appropriate hybridizations. The bonds C(5)—C(5a) and C(10)—C(11) measure 1·477 (3)–1·480 (3) Å; C—C(phenyl) distances are 1·354 (4)–1·408 (7) Å. In the morpholino [and piperidino] rings, C—N = 1·461 (6)–1·466 (3), C—C = 1·512 (4)–1·520 (3), C—O = 1·409 (7) and 1·424 (9) Å; these distances agree with those found in related systems (Carpy, Gadret, Goursolle, Leger & Lehuede, 1979; Andreetti, Bocelli & Sgarabotto, 1979; Destro, 1979; Toupet & Délugeard, 1979; Swaminathan, Sundaralingam, Chattopadhyaya & Reese, 1980). The bond angles C(6)—C(5)=C(10), 124·6 (4) [124·9 (2)]°, and C(5)=C(10)—C(11), 129·2 (4) [129·2 (2)]°, suggest some steric repulsion between the hydrogen atoms bonded to C(6) and C(16); likewise the enlargement of C(4a)—N—C(23), 116·8 (4) [116·5 (2)]°, relative to C(4a)—N—C(27), 113·7 (3) [113·0 (2)]°, indicates steric repulsion, C(23) being situated above the *C* ring of the xanthene. Otherwise bond angles are close to expected values.

Table 4. *Torsion angles* (°) *of interest for DBM*[*DBP*] *with e.s.d.'s in parentheses*

Ring *A*		
C(5)—C(6)—C(7)—C(8)	−59·3 (6)	[−58·8 (3)]
C(6)—C(7)—C(8)—C(8a)	49·4 (6)	[49·0 (3)]
C(7)—C(8)—C(8a)—C(5a)	−18·1 (7)	[−18·0 (3)]
C(8)—C(8a)—C(5a)—C(5)	−4·9 (7)	[−4·7 (3)]
C(8a)—C(5a)—C(5)—C(6)	−4·7 (6)	[−5·2 (3)]
C(5a)—C(5)—C(6)—C(7)	36·7 (6)	[36·3 (3)]
Ring *B*		
O(1)—C(5a)—C(8a)—C(9)	0·7 (7)	[1·0 (3)]
C(5a)—C(8a)—C(9)—C(9a)	−12·7 (6)	[−13·2 (3)]
C(8a)—C(9)—C(9a)—C(4a)	40·0 (5)	[40·6 (2)]
C(9)—C(9a)—C(4a)—O(1)	−56·4 (4)	[−56·3 (2)]
C(9a)—C(4a)—O(1)—C(5a)	46·8 (5)	[46·2 (2)]
C(4a)—O(1)—C(5a)—C(8a)	−19·0 (6)	[−18·7 (3)]
Ring *C*		
C(1)—C(2)—C(3)—C(4)	50·2 (7)	[50·1 (3)]
C(2)—C(3)—C(4)—C(4a)	−55·1 (6)	[−55·0 (3)]
C(3)—C(4)—C(4a)—C(9a)	59·7 (5)	[59·4 (3)]
C(4)—C(4a)—C(9a)—C(1)	−60·3 (5)	[−60·7 (2)]
C(4a)—C(9a)—C(1)—C(2)	56·2 (6)	[57·1 (3)]
C(9a)—C(1)—C(2)—C(3)	−50·7 (7)	[−51·2 (3)]
Morpholino [piperidino] ring		
C(23)—C(24)—O(2)[C(25)]—C(26)	57·4 (8)	[55·1 (3)]
C(24)—O(2)[C(25)]—C(26)—C(27)	−56·2 (7)	[−53·5 (3)]
O(2)[C(25)]—C(26)—C(27)—N	57·6 (7)	[56·9 (3)]
C(26)—C(27)—N—C(23)	−57·7 (6)	[−59·2 (3)]
C(27)—N—C(23)—C(24)	57·5 (7)	[59·7 (3)]
N—C(23)—C(24)—O(2)[C(25)]	−58·9 (8)	[−59·4 (3)]

Intermolecular distances in both structures correspond to normal van der Waals interactions.

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