Schinazi (1988) report the structures of several 3′-azido-3′-deoxythymidine analogues: in some the azido groups have thermal parameters similar to those of the atoms to which they are attached, in others the azido groups show elevated thermal parameters and, in one case two disordered positions, 26° apart, are found for an azido group. In the present structure molecule *A* does not reach this extreme.

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Structures of Two Pseudoisomorphic Derivatives of Pseudoneolongifolol*

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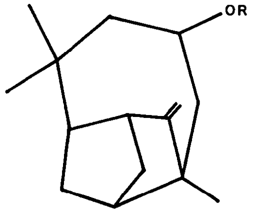
Abstract. $C_{22}H_{27}BrO_2$ (I*a*), pseudoneolongifolyl-*p*-bromobenzoate, $M_r = 403{\cdot}4$, monoclinic, $P2_1$, $a = 7{\cdot}622\,(1)$, $b = 12{\cdot}453\,(1)$, $c = 10{\cdot}433\,(1)$ Å, $\beta = 93{\cdot}81\,(2)°$, $V = 988{\cdot}1\,(2)$ Å^3, $Z = 2$, $D_m = 1{\cdot}37$, $D_x = 1{\cdot}36$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, μ(Mo $K\alpha$) = 2·217 mm^{-1}, $F(000) = 420$, $T = 293$ K, $R = 0{\cdot}055$ for 1009 observed reflections. $C_{22}H_{27}NO_4$ (I*b*), pseudoneolongifolyl-*p*-nitrobenzoate, $M_r = 369{\cdot}5$, triclinic, $P1$, $a = 7{\cdot}569\,(1)$, $b = 10{\cdot}383\,(1)$, $c = 12{\cdot}605\,(1)$ Å, $\alpha = 95{\cdot}52\,(1)$, $\beta = 90{\cdot}19\,(1)$, $\gamma = 94{\cdot}87\,(1)°$, $V = 982{\cdot}3\,(2)$ Å^3, $Z = 2$, $D_m = 1{\cdot}26$, $D_x = 1{\cdot}25$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0{\cdot}042$ mm^{-1}, $F(000) = 396$, $T = 293$ K, $R = 0{\cdot}057$ for 1965 observed reflections. The carbon skeleton (I*a*, I*b*) consists of two eight-membered rings in 'boat-chair' conformation fused to a bicyclo[2.2.1]heptane moiety.

Introduction. Owing to its flexibility, longifolene (decahydro-4,8,8-trimethyl-9-methylene-1,4-methanoazulene) has been used in the preparation of several potential perfumery compounds. In our efforts to analyze conformational flexibility in longifolenes, a study of the silver-ion-assisted solvolysis of 8,11-dibromolongibornane in aqueous acetone resulted in a crystalline compound (I) [m.p. 371 K; 65% yield]. Efforts to obtain crystals suitable for X-ray diffraction studies were futile and hence derivatives (I*a*) and (I*b*) were prepared. Initially crystals of (I*b*) were obtained but attempts to solve the structure failed owing to space-group ambiguity [$P1$ or $P\bar{1}$]. We report here the X-ray structure analyses of (I*a*) and (I*b*).



(I) R = H

(I*a*) $R = \overset{\overset{\large O}{\|}}{C} - PhBr$

(I*b*) $R = \overset{\overset{\large O}{\|}}{C} - PhNO_2$

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Table 1. *Atomic coordinates* (×10⁴) *and equivalent isotropic thermal parameters for non-hydrogen atoms with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{8}{3}\pi^2 \textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j .$$

	x	y	z	B_{eq}(Å²)
(I*a*)				
Br	5693 (3)	2642	9352 (7)	7·61
O(1)	−1450 (14)	−702 (9)	8548 (11)	5·96
O(2)	629 (2)	−1723 (8)	7814 (9)	4·05
C(1)	−3120 (23)	−3044 (14)	5839 (17)	5·37
C(2)	−1433 (18)	−2458 (15)	6184 (13)	4·35
C(3)	−582 (18)	−2628 (11)	7553 (14)	4·00
C(4)	675 (18)	−3581 (12)	7834 (14)	4·00
C(5)	231 (18)	−4712 (12)	7237 (14)	3·98
C(6)	−152 (19)	−4665 (12)	5799 (15)	4·55
C(7)	−1996 (21)	−5052 (13)	5543 (15)	4·67
C(8)	−1960 (23)	−5982 (13)	6513 (16)	5·79
C(9)	−1412 (21)	−5285 (13)	7689 (15)	4·91
C(10)	−2992 (17)	−4545 (13)	7616 (13)	4·45
C(11)	−3278 (16)	−4258 (12)	6166 (13)	4·09
C(12)	−3463 (19)	−2935 (15)	4387 (14)	5·62
C(13)	−4663 (17)	−2456 (19)	6453 (16)	6·12
C(14)	1854 (21)	−5390 (13)	7620 (19)	5·65
C(15)	31 (18)	−838 (13)	8314 (17)	4·57
C(16)	1424 (15)	4 (10)	8548 (11)	2·99
C(17)	886 (17)	1046 (12)	8843 (13)	4·05
C(18)	2177 (15)	1819 (11)	9095 (10)	4·19
C(19)	3946 (24)	1544 (10)	9037 (15)	4·69
C(20)	4418 (15)	546 (13)	8695 (12)	4·27
C(21)	3206 (18)	−246 (11)	8435 (12)	3·91
C(22)	1055 (22)	−4489 (14)	4958 (17)	5·75
I(*b*) Molecule *A*				
N	5586	8946	2428	4·35
O(1)	−1313 (10)	8639 (8)	−583 (5)	5·09
O(2)	774 (8)	7897 (6)	−1723 (5)	3·68
O(3)	7130 (11)	9093 (10)	2160 (7)	7·63
O(4)	5107 (11)	8854 (8)	3328 (6)	5·82
C(1)	−3186 (13)	5756 (9)	−3039 (8)	4·14
C(2)	−1343 (12)	6204 (9)	−2486 (7)	3·79
C(3)	−548 (12)	7580 (9)	−2579 (6)	3·27
C(4)	585 (12)	7828 (9)	−3574 (7)	3·68
C(5)	102 (13)	7183 (9)	−4687 (7)	3·78
C(6)	−260 (13)	5690 (10)	−4725 (7)	4·12
C(7)	−2196 (13)	5361 (11)	−5057 (8)	4·45
C(8)	−2240 (14)	6320 (10)	−5938 (8)	5·22
C(9)	−1673 (13)	7585 (10)	−5212 (7)	4·22
C(10)	−3205 (14)	7525 (10)	−4414 (8)	4·37
C(11)	−3445 (12)	6069 (9)	−4213 (7)	4·11
C(12)	−3531 (15)	4280 (9)	−2978 (9)	5·55
C(13)	−4656 (14)	6447 (11)	−2378 (9)	5·17
C(14)	1662 (14)	7576 (12)	−5417 (9)	5·71
C(15)	169 (15)	8402 (9)	−770 (7)	3·71
C(16)	1628 (11)	8592 (8)	40 (7)	2·83
C(17)	1175 (12)	8805 (8)	1086 (7)	3·43
C(18)	2470 (12)	8949 (8)	1910 (7)	3·12
C(19)	4200 (12)	8893 (8)	1577 (6)	3·03
C(20)	4736 (13)	8740 (9)	552 (7)	3·89
C(21)	3408 (14)	8569 (9)	−261 (7)	3·69
C(22)	943 (14)	4876 (11)	−4627 (8)	5·44
(I*b*) Molecule *B*				
N	−5568 (16)	10744 (10)	6870 (7)	5·11
O(1)	1215 (11)	11389 (8)	3878 (6)	5·33
O(2)	−918 (9)	12126 (7)	2895 (5)	3·79
O(3)	−7068 (14)	11043 (11)	6714 (7)	7·17
O(4)	−5107 (13)	10210 (11)	7639 (7)	8·28
C(1)	3041 (14)	14078 (10)	1729 (9)	4·42
C(2)	1204 (14)	13765 (11)	2277 (7)	4·13
C(3)	341 (14)	12353 (10)	2032 (8)	3·64
C(4)	−852 (12)	12051 (10)	1034 (7)	3·61
C(5)	−410 (14)	12590 (10)	−30 (7)	3·82
C(6)	7 (13)	14093 (10)	94 (6)	3·78
C(7)	1931 (15)	14315 (11)	−214 (9)	4·70
C(8)	1910 (17)	13297 (13)	−1217 (9)	5·64
C(9)	1301 (15)	12137 (11)	−607 (7)	4·34
C(10)	2858 (14)	12211 (10)	164 (8)	4·29
C(11)	3168 (13)	13670 (10)	533 (8)	4·09
C(12)	3403 (15)	15559 (10)	1945 (9)	5·49
C(13)	4478 (14)	13429 (13)	2332 (9)	5·83
C(14)	−2057 (14)	12213 (12)	−749 (8)	5·36
C(15)	−284 (15)	11648 (10)	3754 (8)	3·79
C(16)	−1703 (14)	11461 (9)	4557 (7)	3·39
C(17)	−1179 (16)	11095 (10)	5542 (9)	4·19
C(18)	−2432 (15)	10855 (10)	6324 (8)	4·18
C(19)	−4196 (17)	11002 (10)	6066 (8)	4·07
C(20)	−4741 (14)	11371 (10)	5103 (7)	3·95
C(21)	−3461 (13)	11581 (10)	4320 (7)	3·85
C(22)	−1110 (15)	14953 (11)	326 (8)	5·12

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

I(*a*)

Br—C(19)	1·922 (16)	C(6)—C(7)	1·493 (22)
O(1)—C(15)	1·182 (18)	C(6)—C(22)	1·331 (23)
O(2)—C(3)	1·471 (17)	C(7)—C(8)	1·537 (23)
O(2)—C(15)	1·314 (19)	C(7)—C(11)	1·562 (21)
C(1)—C(2)	1·502 (23)	C(8)—C(9)	1·538 (23)
C(1)—C(11)	1·556 (23)	C(9)—C(10)	1·514 (22)
C(1)—C(12)	1·527 (23)	C(10)—C(11)	1·556 (19)
C(1)—C(13)	1·559 (24)	C(15)—C(16)	1·500 (19)
C(2)—C(3)	1·543 (20)	C(16)—C(17)	1·401 (19)
C(3)—C(4)	1·540 (20)	C(16)—C(21)	1·406 (18)
C(4)—C(5)	1·569 (21)	C(17)—C(18)	1·389 (19)
C(5)—C(6)	1·510 (21)	C(18)—C(19)	1·397 (21)
C(5)—C(9)	1·543 (21)	C(19)—C(20)	1·348 (21)
C(5)—C(14)	1·528 (22)	C(20)—C(21)	1·365 (19)

C(3)—O(2)—C(15)	119·1 (11)	C(8)—C(7)—C(11)	100·8 (12)
C(2)—C(1)—C(11)	119·8 (14)	C(7)—C(8)—C(9)	95·3 (13)
C(2)—C(1)—C(12)	106·4 (14)	C(5)—C(9)—C(8)	101·5 (12)
C(2)—C(1)—C(13)	109·3 (14)	C(5)—C(9)—C(10)	111·2 (12)
C(11)—C(1)—C(12)	107·1 (13)	C(8)—C(9)—C(10)	97·5 (12)
C(11)—C(1)—C(13)	107·2 (13)	C(9)—C(10)—C(11)	104·4 (12)
C(12)—C(1)—C(13)	106·3 (14)	C(1)—C(11)—C(7)	117·7 (12)
C(1)—C(2)—C(3)	117·1 (13)	C(1)—C(11)—C(10)	115·4 (12)
O(2)—C(3)—C(2)	106·6 (11)	C(7)—C(11)—C(10)	102·0 (11)
O(2)—C(3)—C(4)	100·4 (10)	O(1)—C(15)—O(2)	124·3 (15)
C(2)—C(3)—C(4)	120·0 (12)	O(1)—C(15)—C(16)	122·8 (14)
C(3)—C(4)—C(5)	120·1 (12)	O(2)—C(15)—C(16)	112·9 (13)
C(4)—C(5)—C(6)	112·4 (12)	C(15)—C(16)—C(17)	117·9 (12)
C(4)—C(5)—C(9)	116·9 (12)	C(15)—C(16)—C(21)	120·7 (11)
C(4)—C(5)—C(14)	104·0 (12)	C(17)—C(16)—C(21)	121·4 (11)
C(6)—C(5)—C(9)	102·4 (12)	C(16)—C(17)—C(18)	118·0 (12)
C(6)—C(5)—C(14)	112·4 (13)	C(17)—C(18)—C(19)	119·7 (12)
C(9)—C(5)—C(14)	108·9 (12)	Br—C(19)—C(18)	118·5 (11)
C(5)—C(6)—C(7)	106·4 (12)	Br—C(19)—C(20)	120·5 (11)
C(5)—C(6)—C(22)	124·3 (14)	C(18)—C(19)—C(20)	120·8 (14)
C(7)—C(6)—C(22)	128·3 (15)	C(19)—C(20)—C(21)	122·0 (13)
C(6)—C(7)—C(8)	98·6 (13)	C(16)—C(21)—C(20)	117·9 (12)
C(6)—C(7)—C(11)	109·2 (12)		

I(*b*)	Molecule *A*	Molecule *B*
N—O(3)	1·22 (1)	1·22 (2)
N—O(4)	1·20 (1)	1·22 (1)
N—C(19)	1·49 (1)	1·48 (2)
O(1)—C(15)	1·19 (1)	1·20 (1)
O(2)—C(3)	1·46 (1)	1·47 (1)
O(2)—C(15)	1·36 (1)	1·34 (1)
C(1)—C(2)	1·57 (1)	1·58 (2)
C(1)—C(11)	1·56 (1)	1·53 (2)
C(1)—C(12)	1·54 (1)	1·54 (2)
C(1)—C(13)	1·57 (2)	1·56 (2)
C(2)—C(3)	1·52 (1)	1·56 (1)
C(3)—C(4)	1·55 (1)	1·54 (1)
C(4)—C(5)	1·53 (1)	1·53 (1)
C(5)—C(6)	1·55 (1)	1·56 (1)
C(5)—C(9)	1·60 (1)	1·57 (1)
C(5)—C(14)	1·55 (1)	1·54 (1)
C(6)—C(7)	1·52 (1)	1·51 (1)
C(6)—C(22)	1·31 (1)	1·30 (1)
C(7)—C(8)	1·56 (1)	1·57 (1)
C(7)—C(11)	1·59 (1)	1·56 (1)
C(8)—C(9)	1·56 (1)	1·53 (2)
C(9)—C(10)	1·54 (1)	1·52 (1)
C(10)—C(11)	1·55 (1)	1·54 (1)
C(15)—C(16)	1·49 (1)	1·49 (1)
C(16)—C(17)	1·37 (1)	1·40 (1)
C(16)—C(21)	1·40 (1)	1·38 (1)
C(17)—C(18)	1·41 (1)	1·40 (1)
C(18)—C(19)	1·38 (1)	1·40 (2)
C(19)—C(20)	1·36 (1)	1·38 (1)
C(20)—C(21)	1·42 (1)	1·40 (1)

Table 2 (*cont.*)

	Molecule *A*	Molecule *B*
O(3)–N–O(4)	125 (1)	125 (1)
O(3)–N–C(19)	117 (1)	118 (1)
O(4)–N–C(19)	118 (1)	116 (1)
C(3)–O(2)–C(15)	116 (1)	117 (1)
C(2) -C(1)–C(11)	117 (1)	117 (1)
C(2)–C(1)–C(12)	108 (1)	104 (1)
C(2)–C(1)–C(13)	108 (1)	108 (1)
C(11)–C(1)–C(12)	109 (1)	110 (1)
C(11)–C(1)–C(13)	106 (1)	109 (1)
C(12)–C(1)–C(13)	108 (1)	108 (1)
C(1)–C(2)–C(3)	119 (1)	116 (1)
O(2)–C(3)–C(2)	107 (1)	106 (1)
O(2)–C(3)–C(4)	101 (1)	102 (1)
C(2)–C(3)–C(4)	118 (1)	118 (1)
C(3)–C(4)–C(5)	123 (1)	123 (1)
C(4)–C(5)–C(6)	113 (1)	112 (1)
C(4)–C(5)–C(9)	116 (1)	117 (1)
C(4)–C(5)–C(14)	106 (1)	106 (1)
C(6)–C(5)–C(9)	102 (1)	101 (1)
C(6)–C(5)–C(14)	112 (1)	110 (1)
C(9)–C(5)–C(14)	107 (1)	110 (1)
C(5)–C(6)–C(7)	107 (1)	105 (1)
C(5)–C(6)–C(22)	125 (1)	127 (1)
C(7)–C(6)–C(22)	127 (1)	128 (1)
C(6)–C(7)–C(8)	97 (1)	98 (1)
C(6)–C(7)–C(11)	110 (1)	111 (1)
C(8)–C(7)–C(11)	98 (1)	99 (1)
C(7)–C(8)–C(9)	97 (1)	95 (1)
C(5)–C(9)–C(8)	100 (1)	103 (1)
C(5)–C(9)–C(10)	110 (1)	111 (1)
C(8)–C(9)–C(10)	98 (1)	98 (1)
C(9)–C(10)–C(11)	103 (1)	103 (1)
C(1)–C(11)–C(7)	115 (1)	116 (1)
C(1)–C(11)–C(10)	116 (1)	117 (1)
C(7)–C(11)–C(10)	105 (1)	104 (1)
O(1)–C(15)–O(2)	126 (1)	126 (1)
O(1)–C(15)–C(16)	124 (1)	123 (1)
O(2)–C(15)–C(16)	110 (1)	111 (1)
C(15)–C(16)–C(17)	118 (1)	117 (1)
C(15)–C(16)–C(21)	121 (1)	121 (1)
C(17)–C(16)–C(21)	121 (1)	122 (1)
C(16)–C(17)–C(18)	121 (1)	120 (1)
C(17)–C(18)–C(19)	115 (1)	117 (1)
N–C(19)–C(18)	117 (1)	118 (1)
N–C(19)–C(20)	117 (1)	118 (1)
C(18)–C(19)–C(20)	126 (1)	124 (1)
C(19)–C(20)–C(21)	118 (1)	118 (1)
C(16)–C(21)–C(20)	118 (1)	119 (1)

Experimental. (I*a*): Crystal of approximate dimensions $0{\cdot}3 \times 0{\cdot}5 \times 0{\cdot}6$ mm. Density by flotation in KI solution; lattice parameters from 22 reflections ($10 < \theta < 19°$), intensity data collected on Enraf–Nonius CAD-4F-11M single-crystal X-ray diffractometer, graphite-monochromated Mo $K\alpha$ radiation, $\omega/2\theta$ scan mode, scan speed $1°\ \text{min}^{-1}$, $\theta < 23{\cdot}5°$, of 1540 reflections collected ($h = 0$ to 8, $k = 0$ to 14 and $l = -11$ to 11), 1009 were judged significant [$|F_o| > 3\sigma(|F_o|)$], three standard reflections (241, $34\bar{2}$ and $33\bar{2}$) measured every 2000s, 4% variation in intensity, intensities not corrected for absorption, structure solved by direct-methods *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), full-matrix refinement of scale factor, positional and anisotropic thermal parameters (isotropic thermal parameters for H atoms, geometrically fixed) converged to an R of 0·055, $S = 0{\cdot}93$, $(|F_o| - |F_c|)^2$ minimized with unit weights, $(\Delta/\sigma)_{\max} = 0{\cdot}1$, final $\Delta\rho$ excursions $< |0{\cdot}35|$ e Å^{-3}, no correction for secondary extinction, atomic scattering factors from *International Tables for X-ray Crystallography* (1974), *LALS* (Gantzel, Sparks & Trueblood, 1961) used for refinement.

(I*b*): Crystal of approximate dimensions $0{\cdot}4 \times 0{\cdot}1 \times 0{\cdot}8$ mm. Density by flotation in KI solution, lattice parameters for 24 reflections ($8 < \theta < 18°$), intensity data collected on Enraf–Nonius CAD-4F-11M single-crystai X-ray diffractometer, graphite-monochromated Mo $K\alpha$ radiation, $\omega/2\theta$ scan mode, scan speed $1°\ \text{min}^{-1}$, $\theta < 23{\cdot}5°$, out of 2887 reflections collected ($h = 0$ to 8, $k = -11$ to 11 and $l = -14$ to 14) 1965 were judged significant [$|F_o| > 3\sigma(|F_o|)$], three standard reflections (040, 224 and $04\bar{4}$) measured every 2000s, 4% variation in intensity, not corrected for absorption, structure was solved by using the coordinates obtained from (I*a*) (except Br atom); the cell dimensions a, b and c of (I*a*) are interchanged to a, c and b in (I*b*), and the angles α, β and γ in (I*b*) are nearly 90° [$\alpha = 95{\cdot}52$ (1), $\beta = 90{\cdot}19$ (1) and $\gamma = 94{\cdot}87$ (1)°] which results in a pseudoisomorphic situation. A Fourier map based on this assumption gave both molecules of (I*b*). The c axis in (I*b*) behaves like a pseudo-2_1 axis. Full-matrix refinement of scale factor, positional and anisotropic thermal parameters (isotropic thermal parameters for H atoms, geometrically fixed) converged to an R value of 0·057, $(|F_o| - |F_c|)^2$ minimized with unit weights, $(\Delta/\sigma)_{\max} = 0{\cdot}1$, final $\Delta\rho$ excursions $< |0{\cdot}3|$ e Å^{-3}, no correction for secondary extinction, atomic scattering factors from *International Tables for X-ray Crystallography* (1974), *LALS* used for refinement.

Discussion. The atomic parameters with their e.s.d.'s and equivalent isotropic temperature factors are given in Table 1.* Bond lengths and bond angles involving the non-hydrogen atoms for both derivatives are given in Table 2. Perspective views of the two derivatives are shown in Figs. 1 and 2.

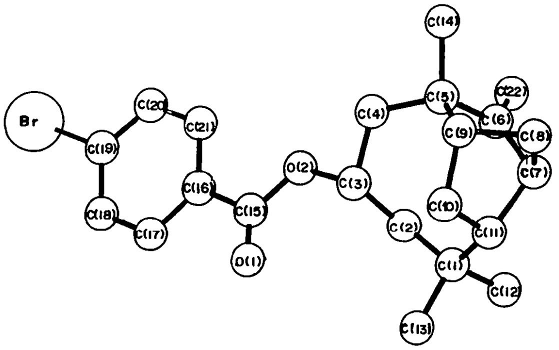

Fig. 1 Perspective view of the molecular structure of compound (I*a*).

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51154 (25 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

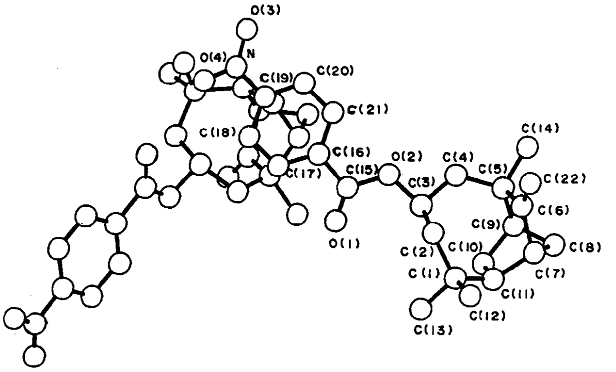

Fig. 2. View of two independent molecules of compound (I*b*) (number of one molecule only shown).

The bond lengths and bond angles of (I*a*) and (I*b*) agree within experimental limits. Indeed, the space-group ambiguity for (I*b*) could be uniquely resolved by comparing the coordinates of the two independent molecules. One molecule is related to the other by the approximate relationship [$-x$, $-y$, $0{\cdot}46 + z$] which deviates significantly from the center of symmetry owing to the arbitrary value of the *z* coordinate. If the *c* axis is taken as unique, the above relation approximates to a 2_1 axis. The angle between the planar rings in the two independent molecules (23·2°) clearly indicates the space group to be the non-centrosymmetric *P*1.

The carbon skeleton in the pseudoneolongifolol moiety consists of two eight-membered rings [C(1), C(2), C(3), C(4), C(5), C(9), C(10), C(11) and C(1), C(2), C(3), C(4), C(5), C(6), C(7), C(11)] having a 'boat-chair' conformation (Bucourt, 1974). The bicyclo[2.2.1]heptane moiety takes the *S*(+,+) conformation (Acharya, Tavale & Guru Row, 1984). The structure is stabilized by van der Waals interactions.

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Structures of 3,5-Bis(benzylidene)-4-piperidone Hydrochloride (I) and its *N*-Methyl Analog (II)

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Abstract. (I): $C_{19}H_{18}NO^+.Cl^-$, $M_r = 311{\cdot}80$, monoclinic, $P2_1/n$, $a = 16{\cdot}787$ (2), $b = 5{\cdot}7373$ (2), $c = 16{\cdot}883$ (1) Å, $\beta = 99{\cdot}07$ (1)°, $V = 1605{\cdot}7$ Å^3, $Z = 4$, D_m(by flotation) = 1·284, $D_x = 1{\cdot}290$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}210$ mm^{-1}, $F(000) = 656$, $T = 287$ K, $R = 0{\cdot}036$ ($wR = 0{\cdot}042$) for 2824 observed reflections. (II): $C_{20}H_{20}NO^+.Cl^-$, $M_r = 325{\cdot}83$, orthorhombic, $Pc2_1b$, $a = 7{\cdot}065$ (2), $b = 12{\cdot}302$ (2), $c = 19{\cdot}354$ (2) Å, $V = 1682{\cdot}3$ Å^3, $Z = 4$, D_m(by flotation) = 1·290, $D_x = 1{\cdot}283$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}196$ mm^{-1}, $F(000) = 688$, $T = 287$ K, $R = 0{\cdot}062$ ($wR = 0{\cdot}060$) for 1582 observed reflections. The heterocyclic rings exhibit a boat conformation in (I) and a chair conformation in (II). The heterocyclic rings in both molecules are flattened in the moiety of C(3)—C(4)—C(5). The bond lengths and angles show good correspondence between the two molecules which, however, differ significantly with respect to torsion angles. In both molecules the steric repulsions between H atoms attached to C(2)/C(6) and those on the phenyl rings cause increases in the bond angles at the C atoms joining the rings and rotations of the phenyl groups out of the mean plane of the piperidone ring.

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