124·2 (3), C—C—C 102·0–107·1 (3) (5-ring), 117·2–127·9 (3–4) (other sp^2), 106·0–113·8 (3–4)° (other sp^3). Intermolecular distances correspond to van der Waals interactions; the shortest are O(1)···O(2) 3·291 (4), O(2)···C(3) 3·145 (5) Å.

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Structure of 2,3,6,7-Dibenzo-4a*β*,8a*β*-dimethyl-4a,5,8,8a-tetrahydro-1,4-naphthoquinone*

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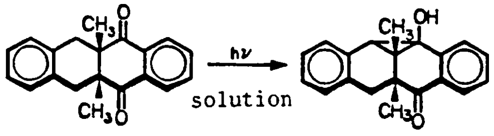
Abstract. $C_{20}H_{18}O_2$, $M_r = 290{\cdot}36$, triclinic, $P\bar{1}$, $a = 9{\cdot}907$ (3), $b = 12{\cdot}094$ (4), $c = 13{\cdot}049$ (4) Å, $\alpha = 80{\cdot}54$ (2), $\beta = 85{\cdot}03$ (2), $\gamma = 89{\cdot}73$ (2)°, $V = 1536{\cdot}3$ (8) Å^3, $Z = 4$ (two molecules per asymmetric unit), $D_x = 1{\cdot}255$ g cm^{-3}, $\lambda(\text{Mo }K\alpha_1) = 0{\cdot}70926$ Å, $\mu = 0{\cdot}71$ cm^{-1}, $F(000) = 616$, $T = 295$ K, final $R = 0{\cdot}046$ for 4388 observed reflections. The crystallographically independent molecules are related by roughly $P2_1/b11$ symmetry, and adopt a similar conformation, with a half-chair cyclohexene ring *cis*-fused to a half-chair cyclohexene-1,4-dione moiety; each molecule is twisted so that the bridgehead methyl groups are staggered with torsion angles of 63 and 65°. The solution and solid-state photochemistry are interpretable in terms of molecular conformation and packing.

Introduction. As part of a study of the photochemistry of various substituted 1,4-naphthoquinone systems it was found that irradiation of the title compound (I) in solution leads to cyclopropanol formation *via* *β*-H-atom abstraction by carbonyl O and closure of the resulting biradical (Ariel, Askari, Scheffer & Trotter, 1986); the title compound is, however, photochemically inert when irradiated in the solid state. The crystal-structure determination of compound (I) has been undertaken in an attempt to resolve the photoreactivity differences in the two media.



(I) (Ia)

Experimental. Crystal size 0·4 × 0·5 × 0·5 mm, m.p. 374–375 K, CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$ radiation, lattice parameters from setting of 23 reflections with $20 \le \theta \le 24°$. 5817 unique reflections with $\theta \le 27°$, h −12→12, k −15→15, l 0→16, ω–2θ scan, ω-scan width $(1{\cdot}0 + 0{\cdot}35\tan\theta)°$, extended 25% on each side for background measurement, horizontal aperture $(2{\cdot}0 + \tan\theta)$ mm, vertical aperture 4 mm, Lp corrections, three standard reflections, no intensity variation. The structure was solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refined by full-matrix least squares using *SHELX*76

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* IUPAC name: 5a*β*,11a*β*-dimethyl-5a,6,11,11a-tetrahydronaphthacene-5,12-dione.

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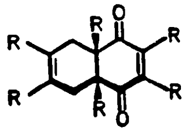
(Sheldrick, 1976) minimizing $\sum w(|F_o| - |F_c|)^2$. All H atoms were located in difference synthesis and refined isotropically. 541 parameters, consisting of 240 positional parameters, 264 anisotropic temperature factors, 36 isotropic temperature factors and a scale factor. Final $R = 0{\cdot}046$, $wR = 0{\cdot}050$ for 4388 reflections for which $F \geq 3\sigma(F)$, where $\sigma^2(I) = S + 2B + [0{\cdot}04(S - B)]^2$, S = scan count, B = time-averaged background count; five strong reflections were given zero weight during refinement. $R = 0{\cdot}069$, $wR = 0{\cdot}051$ for all data, $w = 1/\sigma^2(F)$, $(\Delta/\sigma)_{\max} = 0{\cdot}08$, $\pm 0{\cdot}22$ e Å^{-3} in final difference synthesis, atomic scattering factors from Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965).

Discussion. Final atomic coordinates are in Table 1 (the two molecules listed have arbitrarily been taken with opposite configurations; the crystal is racemic), bond distances, bond angles and selected torsion angles in Table 2.*

The conformation of the molecule (Fig. 1) is twisted about the C(4A)—C(8A) bond, so that the bridgehead methyl groups are staggered, as in the related compound *cis*-2,3,4a,6,7,8a-hexamethyl-4a,5,8,8a-tetrahydro-1,4-naphthoquinone (II) (Phillips & Trotter, 1976). The degree of 'twist' is shown by the torsion angles C(5)—C(4A)—C(8A)—C(1), −58·5 (2), 57·1 (1)°, for molecules *A* and *B*, respectively, and C(4A1)—C(4A)—C(8A)—C(8A1), 63·4 (2), −64·8 (2)°. In (II) the corresponding values for the two angles are −61·4 (5) and 60·0 (6)°, respectively. Bond lengths and bond angles are not significantly different from those in (II), except for the increase in C(2)—C(3) and C(6)—C(7) [1·397 (2), 1·399 (2) *vs* 1·340 (7) Å; and 1·394 (2), 1·394 (2) *vs* 1·323 (7) Å, respectively] resulting from the lower bond order. The C(sp^3)—C(sp^3) bond distances (Table 2) are in the range 1·524 (2)–1·566 (2) Å, mean 1·543 Å. C(4A)—C(8A), 1·558 (2), 1·566 (2) Å, is the longest bond, possibly due to steric effects.



$R=CH_3$

(II)

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* Lists of structure factors, anisotropic thermal parameters and bond distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43258 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atom coordinates* ($\times 10^4$ *for* C, O; $\times 10^3$ *for* H) *and equivalent/isotropic temperature factors* (Å$^2 \times 10^3$)

	Molecule *A*				Molecule *B*			
	x	*y*	*z*	*U*	*x*	*y*	*z*	*U*
O(1)	1489 (1)	362 (1)	1123 (1)	65	4276 (1)	5378 (1)	1164 (1)	54
O(4)	−129 (1)	−2826 (1)	4302 (1)	66	5297 (1)	2214 (1)	4332 (1)	68
C(1)	1025 (1)	−383 (1)	1795 (1)	39	4665 (1)	4637 (1)	1809 (1)	36
C(2)	39 (1)	−126 (1)	2654 (1)	37	5479 (1)	4899 (1)	2649 (1)	37
C(3)	−326 (1)	−948 (1)	3517 (1)	38	5669 (1)	4085 (1)	3517 (1)	39
C(4)	319 (1)	−2069 (1)	3636 (1)	40	4993 (1)	2968 (1)	3651 (1)	42
C(4A)	1583 (1)	−2197 (1)	2911 (1)	36	3910 (1)	2820 (1)	2924 (1)	36
C(4A1)	1936 (2)	−3437 (1)	2970 (2)	54	3570 (2)	1575 (1)	2985 (2)	55
C(5)	2750 (1)	−1571 (1)	3293 (1)	37	2634 (1)	3445 (1)	3284 (1)	39
C(6)	3998 (1)	−1394 (1)	2536 (1)	35	1579 (1)	3594 (1)	2510 (1)	38
C(7)	3934 (1)	−1437 (1)	1480 (1)	38	1906 (1)	3525 (1)	1461 (1)	41
C(8)	2636 (2)	−1721 (2)	1059 (1)	45	3323 (2)	3256 (2)	1057 (1)	45
C(8A)	1359 (1)	−1617 (1)	1782 (1)	37	4405 (1)	3394 (1)	1790 (1)	36
C(8A1)	134 (2)	−2123 (2)	1351 (2)	55	5757 (2)	2915 (2)	1386 (2)	50
C(9)	5227 (2)	−1139 (1)	2892 (1)	45	252 (2)	3848 (1)	2841 (2)	50
C(10)	6379 (2)	−924 (1)	2206 (2)	54	−728 (2)	4028 (1)	2146 (2)	60
C(11)	6321 (2)	−971 (1)	1163 (2)	56	−416 (2)	3937 (2)	1120 (2)	64
C(12)	5115 (2)	−1230 (1)	809 (1)	48	899 (2)	3688 (1)	774 (2)	54
C(13)	−549 (2)	930 (1)	2585 (2)	51	6094 (2)	5950 (1)	2561 (2)	51
C(14)	−1512 (2)	1149 (2)	3355 (2)	59	6903 (2)	6168 (2)	3312 (2)	62
C(15)	−1895 (2)	335 (2)	4192 (2)	61	7103 (2)	5364 (2)	4156 (2)	65
C(16)	−1297 (2)	−703 (2)	4283 (1)	52	6476 (2)	4329 (2)	4272 (1)	56
H(4A1)	282 (2)	−353 (2)	264 (2)	82 (7)	276 (2)	148 (2)	262 (2)	77 (6)
H(4A2)	130 (2)	−382 (2)	263 (2)	71 (6)	342 (2)	124 (2)	375 (2)	77 (6)
H(4A3)	204 (2)	−378 (2)	367 (2)	91 (8)	438 (2)	120 (2)	268 (2)	79 (6)
H(51)	296 (1)	−195 (1)	396 (1)	38 (4)	290 (1)	421 (1)	342 (1)	41 (4)
H(52)	241 (1)	−81 (1)	346 (1)	43 (4)	223 (2)	305 (1)	396 (1)	51 (5)
H(81)	254 (1)	−129 (1)	42 (1)	39 (4)	357 (2)	370 (1)	39 (1)	53 (5)
H(82)	264 (2)	−249 (2)	94 (1)	62 (5)	334 (2)	245 (1)	96 (1)	57 (5)
H(8A1)	32 (2)	−287 (2)	130 (2)	82 (7)	567 (2)	214 (2)	141 (2)	72 (6)
H(8A2)	4 (2)	−175 (2)	70 (2)	63 (6)	648 (2)	300 (2)	180 (2)	69 (6)
H(8A3)	−73 (2)	−211 (1)	181 (2)	66 (5)	602 (2)	329 (2)	66 (1)	53 (5)
H(9)	523 (2)	−116 (1)	366 (1)	53 (5)	6 (2)	391 (1)	357 (2)	62 (5)
H(10)	720 (2)	−72 (1)	247 (1)	57 (5)	−166 (2)	420 (2)	239 (2)	71 (6)
H(11)	715 (2)	−82 (1)	70 (1)	60 (5)	−107 (2)	406 (2)	62 (2)	76 (6)
H(12)	505 (2)	−122 (1)	7 (2)	59 (5)	120 (2)	365 (2)	4 (2)	65 (6)
H(13)	−28 (2)	147 (2)	199 (2)	71 (6)	595 (2)	654 (2)	194 (1)	61 (5)
H(14)	−193 (2)	188 (2)	327 (1)	67 (5)	734 (2)	691 (2)	325 (2)	77 (6)
H(15)	−260 (2)	47 (1)	471 (1)	62 (5)	767 (2)	556 (2)	464 (2)	81 (6)
H(16)	−149 (2)	−127 (2)	489 (2)	64 (5)	652 (2)	373 (2)	488 (2)	81 (6)

The distances between the carbonyl O atoms, O(1), and the β-H atoms H(81), are 2·51 (2) and 2·54 (2) Å for the two molecules of (I), compared to 2·47 (6) Å in (II). Since the van der Waals O···H contact is about 2·72 Å, the photochemical reaction pathway for β-H abstraction from C(8) by O(1) is feasible for both (I) and (II). However, while compound (I) undergoes this photoreaction only in solution and is unreactive in the solid state, compound (II) follows this photorearrangement both in solution and in the solid state (Scheffer, Trotter, Gayler & Bear, 1973; Dzakpasu, Phillips, Scheffer & Trotter, 1976). The other relevant geometric parameters for β-H abstraction by O(1), described by τ (the degree by which β-H lies outside the plane of the carbonyl group), and Δ [the angle C(1)–O(1)···β-H], are: $\tau = 3$, 6° for (I), compared with 0° for (II), and $\Delta = 81$, 81° for (I), compared with 85° for (II). An ideal geometry is described by $\tau = 0°$ and $\Delta = 90°$. The photoproduct for compound (II) involves C(1)···C(6)-bond formation (3·35 Å). However, for (I), C(6) is part of an aromatic ring system, and the solution product results from C(1)···C(8) bonding, distances 2·513 (2) and 2·512 (2) Å.

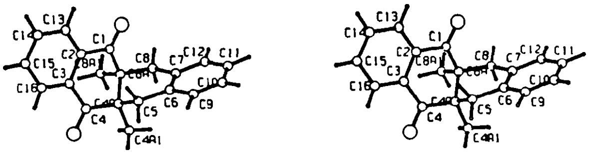

Fig. 1. Stereodiagram of (I) (molecule *A*) with crystallographic atomic labelling.

The lack of photoreactivity in the solid state can be rationalized from the packing arrangement of the molecules in the crystal. The molecules pack in stacks

Table 2. *Bond lengths* (Å), *bond angles* (°), *and selected torsion angles* (°)

	Molecule *A*	Molecule *B*		Molecule *A*	Molecule *B*		Molecule *A*	Molecule *B*
O(1)–C(1)	1·211 (2)	1·210 (2)	C(4A)–C(4A1)	1·530 (2)	1·533 (2)	C(8)–C(8A)	1·529 (2)	1·524 (2)
O(4)–C(4)	1·211 (2)	1·219 (2)	C(4A)–C(5)	1·546 (2)	1·547 (2)	C(8A)–C(8A1)	1·550 (3)	1·542 (2)
C(1)–C(2)	1·493 (2)	1·491 (2)	C(4A)–C(8A)	1·558 (2)	1·566 (2)	C(9)–C(10)	1·385 (2)	1·378 (3)
C(1)–C(8A)	1·529 (2)	1·531 (2)	C(5)–C(6)	1·507 (2)	1·505 (2)	C(10)–C(11)	1·378 (3)	1·369 (4)
C(2)–C(3)	1·397 (2)	1·399 (2)	C(6)–C(7)	1·394 (2)	1·394 (2)	C(11)–C(12)	1·373 (3)	1·390 (3)
C(2)–C(13)	1·394 (2)	1·395 (2)	C(6)–C(9)	1·394 (2)	1·397 (2)	C(13)–C(14)	1·381 (3)	1·377 (3)
C(3)–C(4)	1·488 (2)	1·488 (2)	C(7)–C(8)	1·505 (2)	1·509 (2)	C(14)–C(15)	1·373 (3)	1·372 (3)
C(3)–C(16)	1·394 (2)	1·390 (3)	C(7)–C(12)	1·396 (2)	1·390 (3)	C(15)–C(16)	1·377 (3)	1·380 (3)
C(4)–C(4A)	1·525 (2)	1·523 (2)						
C(2)–C(1)–O(1)	120·4 (1)	120·8 (1)	C(5)–C(4A)–C(4A1)	109·5 (1)	109·6 (1)	C(4A)–C(8A)–C(1)	109·0 (1)	108·0 (1)
C(8A)–C(1)–O(1)	122·4 (1)	122·7 (1)	C(8A)–C(4A)–C(4A1)	112·6 (1)	112·3 (1)	C(8)–C(8A)–C(1)	110·4 (1)	110·6 (1)
C(8A)–C(1)–C(2)	117·1 (1)	116·4 (1)	C(4A1)–C(4A)–C(4)	110·0 (1)	110·4 (1)	C(8A1)–C(8A)–C(1)	106·0 (1)	106·5 (1)
C(3)–C(2)–C(1)	120·4 (1)	120·4 (1)	C(8A)–C(4A)–C(5)	107·9 (1)	107·8 (1)	C(8)–C(8A)–C(4A)	109·7 (1)	109·5 (1)
C(13)–C(2)–C(1)	120·0 (1)	120·2 (1)	C(6)–C(5)–C(4A)	114·1 (1)	113·6 (1)	C(8A1)–C(8A)–C(4A)	112·3 (1)	112·5 (1)
C(13)–C(2)–C(3)	119·6 (1)	119·3 (1)	C(7)–C(6)–C(5)	121·3 (1)	121·6 (1)	C(10)–C(9)–C(6)	120·6 (2)	120·8 (2)
C(4)–C(3)–C(2)	121·0 (1)	120·7 (1)	C(9)–C(6)–C(5)	119·3 (1)	119·3 (1)	C(11)–C(10)–C(9)	120·1 (2)	120·2 (2)
C(16)–C(3)–C(2)	119·2 (1)	119·6 (1)	C(9)–C(6)–C(7)	119·4 (1)	119·1 (1)	C(12)–C(11)–C(10)	119·5 (2)	120·0 (2)
C(16)–C(3)–C(4)	119·7 (1)	119·6 (1)	C(8)–C(7)–C(6)	121·5 (1)	121·5 (1)	C(11)–C(12)–C(7)	121·6 (2)	120·6 (2)
C(4A)–C(4)–C(3)	116·9 (1)	117·4 (1)	C(12)–C(7)–C(6)	118·7 (1)	119·3 (1)	C(14)–C(13)–C(2)	119·9 (2)	120·0 (2)
C(3)–C(4)–O(4)	120·6 (1)	120·3 (1)	C(12)–C(7)–C(8)	119·8 (1)	119·1 (2)	C(15)–C(14)–C(13)	120·6 (2)	120·6 (2)
C(4A)–C(4)–O(4)	122·5 (1)	122·2 (1)	C(8A)–C(8)–C(7)	114·6 (1)	114·3 (1)	C(16)–C(15)–C(14)	120·1 (2)	120·3 (2)
C(5)–C(4A)–C(4)	107·1 (1)	107·3 (1)	C(8A1)–C(8A)–C(8)	109·4 (1)	109·7 (1)	C(15)–C(16)–C(3)	120·5 (2)	120·1 (2)
C(8A)–C(4A)–C(4)	109·6 (1)	109·2 (1)						

	Molecule *A*	Molecule *B*		Molecule *A*	Molecule *B*
O(1)–C(1)–C(2)–C(3)	−169·5 (2)	165·7 (1)	C(4A1)–C(4A)–C(8A)–C(1)	−179·5 (1)	177·9 (1)
O(1)–C(1)–C(2)–C(13)	12·1 (2)	−16·3 (2)	C(4A1)–C(4A)–C(8A)–C(8)	−58·5 (2)	57·5 (2)
C(8A)–C(1)–C(2)–C(3)	13·3 (2)	−16·5 (2)	C(4A1)–C(4A)–C(8A)–C(8A1)	63·4 (2)	−64·8 (2)
C(8A)–C(1)–C(2)–C(13)	−165·2 (1)	161·5 (1)	C(5)–C(4A)–C(8A)–C(1)	−58·5 (2)	57·1 (1)
O(1)–C(1)–C(8A)–C(4A)	138·8 (2)	−134·4 (1)	C(5)–C(4A)–C(8A)–C(8)	62·5 (2)	−63·4 (2)
O(1)–C(1)–C(8A)–C(8)	18·2 (2)	−14·6 (2)	C(5)–C(4A)–C(8A)–C(8A1)	−175·7 (1)	174·4 (1)
O(1)–C(1)–C(8A)–C(8A1)	−100·2 (2)	104·5 (2)	C(4A)–C(5)–C(6)–C(7)	20·8 (2)	−20·3 (2)
C(2)–C(1)–C(8A)–C(4A)	−44·1 (2)	47·8 (2)	C(4A)–C(5)–C(6)–C(9)	−161·9 (1)	162·1 (1)
C(2)–C(1)–C(8A)–C(8)	−164·7 (1)	167·7 (1)	C(5)–C(6)–C(7)–C(8)	−3·3 (2)	2·3 (2)
C(2)–C(1)–C(8A)–C(8A1)	77·0 (2)	−73·3 (2)	C(5)–C(6)–C(7)–C(12)	177·9 (1)	−178·9 (2)
C(1)–C(2)–C(3)–C(4)	3·9 (2)	−3·9 (2)	C(9)–C(6)–C(7)–C(8)	179·3 (2)	−179·9 (2)
C(2)–C(3)–C(4)–O(4)	−169·6 (2)	170·4 (2)	C(9)–C(6)–C(7)–C(12)	0·6 (2)	−1·3 (2)
C(2)–C(3)–C(4)–C(4A)	12·6 (2)	−10·5 (2)	C(5)–C(6)–C(9)–C(10)	−177·2 (2)	177·8 (2)
C(16)–C(3)–C(4)–O(4)	11·3 (2)	−10·8 (2)	C(7)–C(6)–C(9)–C(10)	0·2 (2)	0·1 (3)
C(16)–C(3)–C(4)–C(4A)	−166·6 (1)	168·3 (2)	C(6)–C(7)–C(8)–C(8A)	17·0 (2)	−16·3 (2)
O(4)–C(4)–C(4A)–C(4A1)	14·2 (2)	−14·5 (2)	C(12)–C(7)–C(8)–C(8A)	−164·3 (2)	164·9 (2)
O(4)–C(4)–C(4A)–C(5)	−104·7 (2)	104·9 (2)	C(6)–C(7)–C(12)–C(11)	−1·1 (3)	1·2 (3)
O(4)–C(4)–C(4A)–C(8A)	138·5 (2)	−138·5 (2)	C(8)–C(7)–C(12)–C(11)	−179·9 (2)	180·0 (2)
C(3)–C(4)–C(4A)–C(4A1)	−167·9 (1)	166·4 (1)	C(7)–C(8)–C(8A)–C(1)	73·4 (2)	−72·1 (2)
C(3)–C(4)–C(4A)–C(5)	73·1 (2)	−74·2 (2)	C(7)–C(8)–C(8A)–C(4A)	−46·8 (2)	46·9 (2)
C(3)–C(4)–C(4A)–C(8A)	−43·7 (2)	42·4 (2)	C(7)–C(8)–C(8A)–C(8A1)	−170·3 (2)	170·8 (1)
C(4)–C(4A)–C(5)–C(6)	−167·4 (1)	167·3 (1)	C(6)–C(9)–C(10)–C(11)	−0·6 (3)	1·3 (3)
C(4A1)–C(4A)–C(5)–C(6)	73·4 (2)	−72·7 (2)	C(9)–C(10)–C(11)–C(12)	0·0 (3)	−1·4 (3)
C(8A)–C(4A)–C(5)–C(6)	−49·5 (2)	−49·8 (2)	C(10)–C(11)–C(12)–C(7)	0·7 (3)	0·2 (3)
C(4)–C(4A)–C(8A)–C(1)	57·7 (2)	−59·2 (1)	C(2)–C(13)–C(14)–C(15)	0·2 (3)	−0·6 (3)
C(4)–C(4A)–C(8A)–C(8)	178·8 (1)	−179·7 (1)	C(13)–C(14)–C(15)–C(16)	1·5 (3)	−1·1 (3)
C(4)–C(4A)–C(8A)–C(8A1)	−59·4 (2)	58·1 (2)	C(14)–C(15)–C(16)–C(3)	−1·6 (3)	1·9 (3)

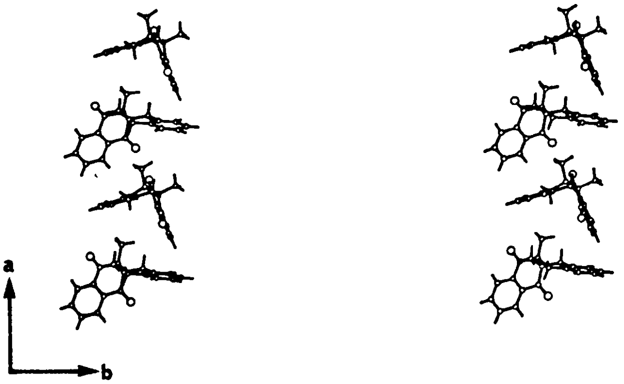

Fig. 2. Stereodiagram of molecular stack consisting of alternating A and B molecules.

consisting of alternating A and B molecules (Fig. 2). A notable feature is that a methyl group of a lower molecule projects directly into the space between the two aromatic rings of an upper molecule. Cyclopropanol formation requires that the two aromatic rings move considerably closer together, and this is prevented by the presence of the methyl group. The γ-H-atom abstraction by an enone C atom [C(2) or C(3)] observed for compound (II) is not possible for compound (I) since C(2) and C(3) are part of an aromatic ring system.

Intermolecular distances correspond to van der Waals contacts. The independent molecules are related by approximate $P2_1/b11$ symmetry, with a pseudo screw axis parallel to **a** at $y\ \frac{1}{4}$, z 0, and pseudo b-glide plane perpendicular to **a** at x 0·275.

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Structure of 2-(*p*-Toluenesulfonyl)-1,2,3,4-tetrahydroisoquinoline

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Abstract. $C_{16}H_{17}NO_2S$, $M_r = 287·4$, monoclinic, $P2_1$, $a = 8·234$ (2), $b = 6·135$ (1), $c = 14·479$ (2) Å, $\beta = 94·56$ (1)°, $V = 729·1$ (2) Å^3, $Z = 2$, $D_m = 1·24$, $D_x = 1·31$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ(Mo $K\alpha$) = 2·11 mm^{-1}, $F(000) = 304$, room temperature, $R = 0·065$ for 1209 observed reflexions. The heterocyclic fragment of the molecule exhibits a half-chair conformation. The N atom shows considerable pyramidization [sum of valency angles = 343·2 (9)°]. Bond lengths and angles in the aromatic rings do not deviate significantly from standard values.

Introduction. This work is a continuation of our studies of the structures of Reissert compounds (Reissert, 1905) and their analogs. The present compound is a product of reductive decyanation of the corresponding Reissert analog in alkaline solution.

Experimental. Crystals obtained from methanol, colorless prisms. Space group from Weissenberg photographs. Crystal 0·3 × 0·4 × 0·6 mm. D_m by flotation. Syntex $P2_1$ diffractometer, θ–2θ scan. Cell parameters from least-squares treatment of setting angles of 15 reflexions with $15 \leq 2\theta \leq 20°$. No absorption or extinction correction. Profile analysis

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