Both 2-amino groups not only donate both of their protons in hydrogen bonds but also appear to act as proton acceptors for additional hydrogen bonds: the N(7′)···N(2), H(71′)···N(2), N(7)···N(2′) and H(71)···N(2′) contacts are all short. The sum of bond angles at N(2) and N(2′) is 10–13° less than 360°, suggesting some pyramidalization. Pyramidalized amino groups participating in hydrogen bonds as proton acceptors as well as donors have been previously observed in similar triamino compounds: 2,4,6-triamino-5-chloroquinazoline (Rogan & Williams, 1980) and 2,4,6-triaminopyrimidine (Schwalbe & Williams, 1982). The remaining proton donor and acceptor sites at N(4) and N(5) do not hydrogen bond together; instead the N(4) and N(4′) amino groups with H atoms in one set of alternative positions H(41), H(43), H(41′) and H(43′) enter into weak hydrogen-bond-like interactions with N(8), N(7), N(8′) and N(7′) respectively. The alternative coherent set of H-atom positions H(42), H(44), H(42′) and H(44′) does not show this degree of H···N interactions.

Pteridine rings of like kind stack around centers of inversion (Fig. 2). Somewhat surprisingly, the closest contacts are between C atoms with similar substituents: thus C(4)···C(7) and C(4′)···C(7′) are 3·465 (7) and 3·455 (7) Å, respectively. Unprimed phenyl rings are roughly parallel to primed pteridine rings [3·2 (1)° angle between phenyl and pyrazine least-squares planes] and *vice versa* [6·2 (1)° angle].

We thank Smith Kline & French Laboratories, Welwyn Garden City, England, for the sample, Dr T. F. Koetzle for helpful discussions, the Chemistry Department of Brookhaven National Laboratory for financial support for CHS, and the US National Institutes of Health for support under grant No. GM24385. Computations were carried out at the University of Manchester Regional Computer Centre.

References

BONDI, A. (1964). *J. Phys. Chem.* **68**, 441–451.

CHATAR SINGH (1965). *Acta Cryst.* **19**, 861–864.

CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

MAIN, P., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO78.* A program for plotting molecular and crystal structures. Univ. of Cambridge, England.

OSDENE, T. S., RUSSELL, P. B. & RANE, L. (1967). *J. Med. Chem.* **10**, 431–434.

PHILLIPS, T. & BRYAN, R. F. (1969). *Acta Cryst.* A**25**, S200.

ROGAN, P. K. & WILLIAMS, G. J. B. (1980). *Acta Cryst.* B**36**, 2358–2362.

SCHWALBE, C. H. & CODY, V. (1983). *Chemistry and Biology of Pteridines*, edited by J. A. BLAIR, pp. 511–515. Berlin: de Gruyter.

SCHWALBE, C. H. & WILLIAMS, G. J. B. (1982). *Acta Cryst.* B**38**, 1840–1843.

SCHWALBE, C. H. & WILLIAMS, G. J. B. (1986*a*). *Acta Cryst.* C**42**, 1252–1254.

SCHWALBE, C. H. & WILLIAMS, G. J. B. (1986*b*). *Acta Cryst.* C**42**, 1254–1257.

SHELDRICK, G. M. (1976). *SHELX76.* Program for crystal structure determination. Univ. of Cambridge, England.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

TAYLOR, R. & KENNARD, O. (1986). *Acta Cryst.* B**42**, 112–120.

Acta Cryst. (1987). C**43**, 1100–1103

Structure of (6,7)-Benzo-2,3,4α,4aβ,8aβ-pentamethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4β-ol*

BY SARA ARIEL AND JAMES TROTTER

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

(*Received* 23 *July* 1986; *accepted* 5 *January* 1987)

Abstract. $C_{19}H_{24}O_2$, $M_r = 284{\cdot}40$, monoclinic, $P2_1/c$, $a = 12{\cdot}2068\ (7)$, $b = 7{\cdot}6627\ (5)$, $c = 17{\cdot}3623\ (15)$ Å, $\beta = 105{\cdot}290\ (6)°$, $V = 1566{\cdot}5\ (2)$ Å^3, $Z = 4$, $D_x = 1{\cdot}206$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 5{\cdot}6$ cm^{-1}, $F(000) = 616$, $T = 295$ K, $R = 0{\cdot}069$ for 1454 observed reflections. The conformation of the molecule is twisted such that the bridgehead methyl groups are staggered with a torsion angle of 64·9°. Bond lengths and angles are close to normal values. Despite the *syn* hydroxyl group, the bulkier methyl causes the molecule to adopt a conformation typical of OH-*anti* derivatives. Molecules in the crystal are linked by hydrogen bonds between symmetry-related molecules with

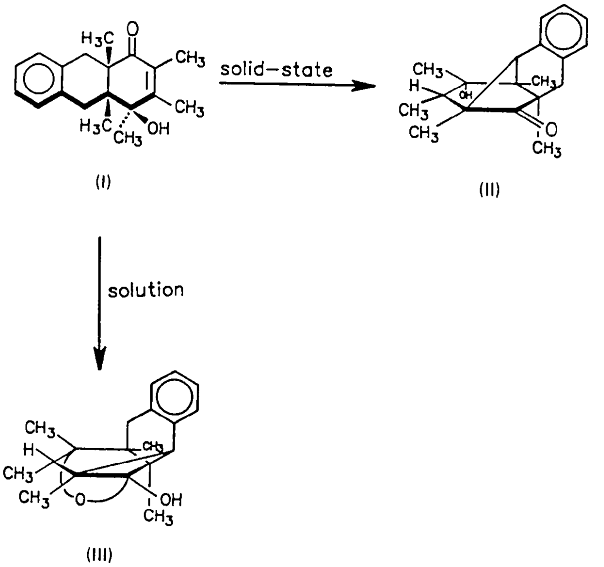
---

* IUPAC name: 4β-hydroxy-2,3,4α,4aβ,9aβ-pentamethyl-*cis*-4aβ,9,9aβ,10-tetrahydro-1(4*H*)-anthracenone.

0108-2701/87/061100-04$01.50

O(1)···O(2) = 2·885 Å. The photochemical reaction in the solid state is accounted for on the basis of the molecular geometry.

Introduction. Solid-state/solution photoreactivity differences have been observed in various substituted tetrahydronaphthoquinols (Appel, Greenhough, Scheffer, Trotter & Walsh, 1980). In the case of the present compound (I), photolysis of its crystals gives compound (II), while photolysis in solution gives compound (III). The crystal structure of (I) was determined in order to explain the behaviour in the solid state.

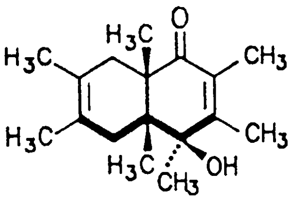


(I) (II) (III)

Experimental. Crystal size 0·2 × 0·2 × 0·2 mm, m.p. 444–445 K, Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Cu $K\alpha$ radiation, lattice parameters from setting of 25 reflections with $25 \leq \theta \leq 40°$, 2508 unique reflections with $\theta \leq 75°$, $h = -15 \to 15$, $k = 0 \to 9$, $l = 0 \to 21$; ω–$\frac{1}{3}\theta$ scan, ω scan width $(0·90 + 0·14\tan\theta)°$, extended 25% on each side for background measurement, horizontal aperture $(1·0 + \tan\theta)$ mm, vertical aperture 4 mm, Lp corrections, three standard reflections. Structure was solved by direct methods with *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refined by full-matrix least squares minimizing $\sum w(|F_o| - |F_c|)^2$ using *SHELX*76 (Sheldrick, 1976). Except for the hydroxyl hydrogen (located in a difference synthesis), all hydrogens were put in calculated positions, and methyl hydrogens were then refined as rigid groups possessing a local C_3 symmetry. The temperature factors of all H atoms were refined isotropically. 232 parameters consisting of 81 positional parameters, 126 anisotropic temperature factors, 24 isotropic temperature factors, and a scale factor. Convergence at $R = 0·069$, $wR = 0·048$ for 1454 observed reflections for which $F \geq 3\sigma(F)$, where $\sigma^2(I) = S + 2B + [0·04(S-B)]^2$, S = scan count, B = time-averaged background count. $R = 0·135$, $wR = 0·064$ for all data, $w = 1/\sigma^2(F)$, $(\Delta/\sigma)_{max} = 0·2$, $\pm 0·27$ e Å^{-3} in final difference synthesis, atomic scattering factors from Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965). No corrections for absorption or secondary extinction.

Discussion. Final atomic coordinates are in Table 1, bond distances, bond angles, and selected torsion angles in Table 2.*

The molecular conformation of the title compound (Fig. 1) is twisted about the C(4*A*)—C(8*A*) bond, so that the bridgehead methyl groups are staggered, as in the related compound 2,3,4α,4aβ,6,7,8aβ-heptamethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4β-ol (IV) (Secco & Trotter, 1982*a*). The degree of 'twist' is shown by the torsion angles C(5)—C(4*A*)—C(8*A*)—C(1), 59·2 (3), and C(4*A*1)—C(4*A*)—C(8*A*)—C(8*A*1), −64·9 (4)°. In (IV) the corresponding values for the two angles are 62·2 (2) and −62·7 (2)°, respectively. Bond lengths and bond angles are not significantly different from those in (IV), except for the increase in C(6)—C(7), 1·388 (4) *vs.* 1·316 (3) Å, resulting from the lower bond order. The C(sp^3)—C(sp^3) bond distances (Table 2) are in the range 1·530 (5)–1·569 (5) Å, mean 1·546 Å. C(4)—C(4*A*) is relatively long, 1·569 (5) Å, because of steric effects due to the methyl groups on C(4) and C(4*A*).



(IV)

Molecules of (I) crystallize with the conformation common to all naphthoquinols studied, in which the bulkier substituent on C(4) assumes the pseudo-equatorial position (Secco & Trotter, 1982*a*). Although the 4-OH is *syn*† to the bridgehead methyl groups, the conformation adopted (Fig. 1) is characteristic of the naphthoquinols which have the hydroxyl group *anti* to the bridgehead substituents, *i.e.* a half-chair cyclo-

---

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, and bond distances and angles involving hydrogen atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43701 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

† *cis* (or *trans*) is used here to specify the configuration of ring junction, and *syn* (or *anti*) to specify relation between the methyl substituents at the ring junction and C(4) substituents.

Table 1. *Atom coordinates* (× 10^4) *and temperature factors* (Å^2 × 10^3)

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

	x	y	z	$U_{\rm eq}$
O(1)	1658 (2)	−804 (3)	4437 (2)	60
O(2)	1363 (2)	5623 (4)	3895 (2)	58
C(1)	1669 (3)	791 (5)	4362 (2)	38
C(2)	1598 (3)	1939 (5)	5027 (2)	43
C(21)	1252 (4)	1072 (7)	5714 (2)	67
C(3)	1800 (3)	3670 (5)	4996 (2)	44
C(31)	1594 (4)	4899 (7)	5628 (3)	71
C(4)	2253 (3)	4509 (4)	4353 (2)	41
C(41)	3290 (4)	5654 (6)	4745 (3)	60
C(4A)	2554 (3)	3147 (4)	3765 (2)	33
C(4A1)	2659 (4)	4049 (5)	3002 (2)	53
C(5)	3717 (3)	2315 (4)	4177 (2)	38
C(6)	4023 (3)	743 (4)	3739 (2)	36
C(7)	3199 (3)	−154 (4)	3174 (2)	36
C(8)	1972 (3)	334 (5)	2997 (2)	42
C(8A)	1669 (3)	1656 (4)	3577 (2)	33
C(8A1)	437 (3)	2255 (5)	3200 (2)	48
C(9)	5154 (3)	208 (5)	3904 (2)	46
C(10)	5472 (4)	−1193 (5)	3505 (2)	56
C(11)	4655 (4)	−2050 (5)	2916 (2)	56
C(12)	3531 (4)	−1539 (5)	2761 (2)	46

hexene ring *cis*-fused to a half-chair cyclohexenone moiety, with the bulkier 4-methyl substituent pseudo-equatorial. The spatial consequence of this arrangement is the proximity of the β-enone carbon, C(3), to H(51) (2·80 Å). Furthermore, the angle between the C(3)···H(51) vector and its projection on the plane of the C(3)=C(2) double bond [C(1), C(2), C(3), C(4)], τ, and the angle between the C(3)···H(51) and the C(3)=C(2) vectors, Δ, are 48 and 72°, respectively. This geometry is highly favourable for H-abstraction by the β-enone C, which is observed in the solid-state photolysis. The corresponding values for the C(3)···H1(5) distance, τ, and Δ for compound (IV) are 2·81 (2) Å, 50 and 78·3 (4)°, respectively, allowing the corresponding H-abstraction by the β-enone C photolysis to occur in the solid state (Jiang, Scheffer, Secco & Trotter, 1981).

The distance between the carbonyl oxygen, O(1), and the β-hydrogen, H(82), is 2·44 Å, compared with 2·41 (2) Å in (IV). Since the van der Waals O···H contact is about 2·7 Å, the photochemical reaction pathway for β-hydrogen abstraction from C(8) by O(1) is feasible for both (I) and (IV). The other relevant geometric parameters for β-hydrogen abstraction by O(1), described by τ [the degree by which H(β) lies outside the plane of the carbonyl group], and Δ [the angle C(1)—O(1)···H(β)], are $\tau = 7°$, $\Delta = 96°$ for (I), compared with $\tau = 1°$, $\Delta = 83°$ for (IV). Thus in both cases there is an almost perfect alignment for the β-H with the non-bonding orbital of O(1). However, it was argued in previous work on tetrahydronaphthoquinols (Secco & Trotter, 1982*b*) that substituents on the C(2) and C(3) positions of the cyclohexenone moiety play a critical role in determining the photochemical reaction pathway, possibly by lowering the energy of the (π,π^*) transition state from which the C abstraction of the γ-H is considered to originate. The lack of β-H abstraction by O in this system, as well as for compound (IV), supports the above argument but does not clarify the role of the C(2) and C(3) substituents.

The result of the photochemical reactivity preference is that compound (I) when photolyzed in the solid state undergoes γ-H, H(51), abstraction by β-enone carbon, C(3), followed by C(2)···C(5) bonding [C(2)···C(5) distance is 3·313 (5) Å] to form keto-alcohol (II). The solution photoproduct (III) is formed from a higher-energy ring-flipped conformer of compound (I) which brings one hydrogen atom on C(8) to the proximity of the enone moiety. γ-Hydrogen abstraction by C(3) is followed by C(2)···C(8) bonding and cyclization of the resulting keto-alcohol (which could not be isolated in the solution phase) generates hemiacetal (III).

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

C(1)—O(1)	1·230 (5)	C(6)—C(7)	1·388 (4)
C(1)—C(2)	1·473 (5)	C(7)—C(8)	1·495 (5)
C(2)—C(21)	1·519 (6)	C(8)—C(8A)	1·540 (5)
C(2)—C(3)	1·353 (5)	C(1)—C(8A)	1·515 (5)
C(3)—C(31)	1·516 (6)	C(4A)—C(8A)	1·547 (5)
C(3)—C(4)	1·514 (6)	C(8A)—C(8A1)	1·543 (5)
C(4)—O(2)	1·444 (4)	C(6)—C(9)	1·396 (5)
C(4)—C(41)	1·543 (5)	C(9)—C(10)	1·388 (6)
C(4)—C(4A)	1·569 (5)	C(10)—C(11)	1·391 (5)
C(4A)—C(4A1)	1·530 (5)	C(11)—C(12)	1·382 (6)
C(4A)—C(5)	1·548 (5)	C(7)—C(12)	1·399 (5)
C(5)—C(6)	1·523 (5)	H(2)—O(2)	0·96 (6)

C(2)—C(1)—O(1)	120·4 (3)	C(8A)—C(4A)—C(4A1)	111·4 (3)
C(8A)—C(1)—O(1)	122·2 (3)	C(6)—C(5)—C(4A)	114·3 (3)
C(8A)—C(1)—C(2)	117·3 (3)	C(7)—C(6)—C(5)	121·2 (3)
C(21)—C(2)—C(1)	116·1 (3)	C(9)—C(6)—C(5)	119·3 (3)
C(3)—C(2)—C(1)	120·3 (3)	C(9)—C(6)—C(7)	119·6 (3)
C(3)—C(2)—C(21)	123·5 (4)	C(8)—C(7)—C(6)	121·4 (3)
C(4)—C(3)—C(2)	123·5 (3)	C(12)—C(7)—C(6)	118·9 (3)
C(31)—C(3)—C(2)	120·9 (4)	C(12)—C(7)—C(8)	119·7 (3)
C(4)—C(3)—C(31)	115·6 (3)	C(8A)—C(8)—C(7)	115·5 (3)
C(3)—C(4)—O(2)	106·8 (3)	C(8)—C(8A)—C(1)	110·9 (3)
C(41)—C(4)—O(2)	108·5 (3)	C(8A1)—C(8A)—C(1)	106·3 (3)
C(41)—C(4)—C(3)	109·4 (3)	C(8A1)—C(8A)—C(8)	107·1 (3)
C(4A)—C(4)—O(2)	107·9 (3)	C(4A)—C(8A)—C(1)	107·4 (3)
C(4A)—C(4)—C(3)	113·0 (3)	C(8)—C(8A)—C(4A)	110·4 (3)
C(4A)—C(4)—C(41)	111·1 (3)	C(8A1)—C(8A)—C(4A)	114·7 (3)
C(5)—C(4A)—C(4)	108·5 (3)	C(10)—C(9)—C(6)	121·0 (4)
C(8A)—C(4A)—C(4)	111·0 (3)	C(11)—C(10)—C(9)	119·5 (4)
C(8A)—C(4A)—C(5)	107·3 (3)	C(12)—C(11)—C(10)	119·4 (4)
C(4A1)—C(4A)—C(4)	110·5 (3)	C(11)—C(12)—C(7)	121·5 (4)
C(5)—C(4A)—C(4A1)	108·1 (3)		

O(1)—C(1)—C(2)—C(21)	−13·1 (5)	C(3)—C(4)—C(4A)—C(8A)	38·9 (4)
O(1)—C(1)—C(2)—C(3)	169·0 (4)	C(41)—C(4)—C(4A)—C(4A1)	−73·6 (4)
C(8A)—C(1)—C(2)—C(21)	162·6 (3)	C(41)—C(4)—C(4A)—C(5)	44·7 (4)
C(8A)—C(1)—C(2)—C(3)	−15·4 (5)	C(41)—C(4)—C(4A)—C(8A)	162·4 (3)
O(1)—C(1)—C(8A)—C(4A)	−135·8 (4)	C(4)—C(4A)—C(5)—C(6)	169·7 (3)
O(1)—C(1)—C(8A)—C(8)	−15·1 (5)	C(4A1)—C(4A)—C(5)—C(6)	−70·5 (4)
O(1)—C(1)—C(8A)—C(8A1)	100·9 (4)	C(8A)—C(4A)—C(5)—C(6)	49·7 (4)
C(2)—C(1)—C(8A)—C(4A)	48·6 (4)	C(4)—C(4A)—C(8A)—C(1)	−59·2 (4)
C(2)—C(1)—C(8A)—C(8)	169·3 (3)	C(4)—C(4A)—C(8A)—C(8)	179·8 (3)
C(2)—C(1)—C(8A)—C(8A1)	−74·7 (4)	C(4)—C(4A)—C(8A)—C(8A1)	58·6 (4)
C(1)—C(2)—C(3)—C(4)	−8·3 (6)	C(4A1)—C(4A)—C(8A)—C(1)	177·2 (3)
C(2)—C(3)—C(4)—O(2)	114·0 (4)	C(4A1)—C(4A)—C(8A)—C(8)	56·2 (4)
C(2)—C(3)—C(4)—C(41)	−128·8 (4)	C(4A1)—C(4A)—C(8A)—C(8A1)	−64·9 (4)
C(2)—C(3)—C(4)—C(4A)	−4·5 (5)	C(5)—C(4A)—C(8A)—C(1)	59·2 (3)
C(31)—C(3)—C(4)—O(2)	−67·0 (4)	C(5)—C(4A)—C(8A)—C(8)	−61·9 (3)
C(31)—C(3)—C(4)—C(41)	50·3 (5)	C(5)—C(4A)—C(8A)—C(8A1)	177·0 (3)
C(31)—C(3)—C(4)—C(4A)	174·6 (3)	C(4A)—C(5)—C(6)—C(7)	−18·4 (5)
O(2)—C(4)—C(4A)—C(4A1)	45·2 (4)	C(4A)—C(5)—C(6)—C(9)	161·0 (3)
O(2)—C(4)—C(4A)—C(5)	163·5 (3)	C(6)—C(7)—C(8)—C(8A)	−10·2 (5)
O(2)—C(4)—C(4A)—C(8A)	−78·9 (3)	C(7)—C(8)—C(8A)—C(1)	−75·6 (4)
C(3)—C(4)—C(4A)—C(4A1)	163·0 (3)	C(7)—C(8)—C(8A)—C(4A)	43·3 (4)
C(3)—C(4)—C(4A)—C(5)	−78·8 (4)	C(7)—C(8)—C(8A)—C(8A1)	168·9 (3)

Hydrogen bonding, found in all the naphthoquinols studied, is present in this structure as O(2)—H(2)···O(1) interactions linking molecules along the *b* axis (Fig. 2): O···O = 2·885 (5), H···O = 1·97 Å, O—H···O = 160°.

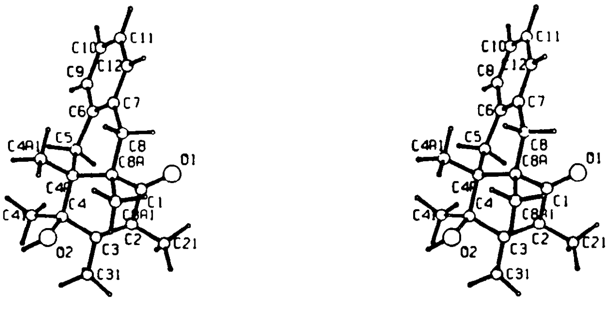


Fig. 1. Stereoscopic view of (I) with crystallographic atomic labelling.

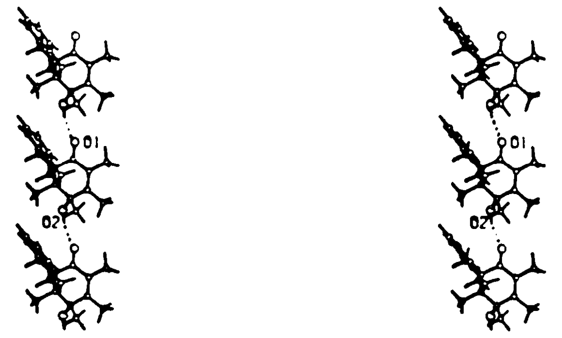


Fig. 2. Stereoscopic view of the H-bonding arrangement of (I).

Acknowledgement is made to Professor J. R. Scheffer and Mr S. H. Askari for their collaborative studies on the solid-state photochemistry, the Natural Sciences and Engineering Research Council of Canada for financial support, and the University of British Columbia Computing Centre for assistance.

References

Appel, W. K., Greenhough, T. J., Scheffer, J. R., Trotter, J. & Walsh, L. (1980). *J. Am. Chem. Soc.* **102**, 1158–1161.
Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* A**24**, 321–324.
Jiang, Z. Q., Scheffer, J. R., Secco, A. S. & Trotter, J. (1981). *Tetrahedron Lett.* **22**, 891–894.
Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.
Secco, A. S. & Trotter, J. (1982*a*). *Acta Cryst.* B**38**, 2190–2196.
Secco, A. S. & Trotter, J. (1982*b*). *Acta Cryst.* B**38**, 1233–1237.
Sheldrick, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
Stewart, R. F., Davidson, E. R. & Simpson, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

Acta Cryst. (1987). C**43**, 1103–1105

Structure of (6,7)-Benzo-2,3,4a*β*,8a*β*-tetramethyl-4a,5,8,8a-tetrahydro-1-naphthoquin-4*β*-yl Acetate*

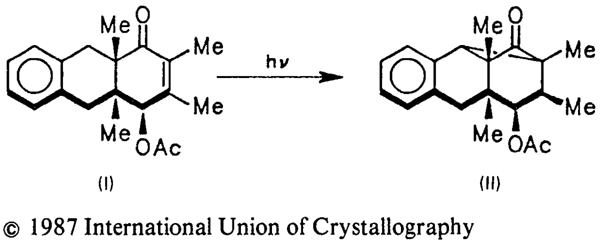
By Sara Ariel and James Trotter

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

(*Received* 23 *July* 1986; *accepted* 6 *January* 1987)

Abstract. $C_{20}H_{24}O_3$, $M_r = 312\cdot41$, triclinic, $P\bar{1}$, $a = 9\cdot4624\ (6)$, $b = 9\cdot7485\ (7)$, $c = 10\cdot6743\ (7)$ Å, $\alpha = 66\cdot641\ (5)$, $\beta = 79\cdot664\ (6)$, $\gamma = 70\cdot336\ (6)°$, $V = 850\cdot0\ (1)$ Å^3, $Z = 2$, $D_x = 1\cdot220$ g cm^{-3}, $\lambda(\text{Cu}\ K\alpha) = 1\cdot5418$ Å, $\mu = 5\cdot963$ cm^{-1}, $F(000) = 336$, $T = 295$ K, $R = 0\cdot051$ for 2391 observed reflections. The conformation of the molecule is twisted such that the bridgehead methyl groups are staggered with a torsion angle of 60·8°. Bond lengths and angles are close to normal values. The photochemical reaction in the solid state is accounted for on the basis of the molecular geometry.

Introduction. Irradiation of compound (I), whether in solution or in the solid state, gives compound (II). The reaction is initiated by intramolecular allylic H-atom transfer to the *β*-carbon atom of the enone moiety. The crystallographic study of (I) was undertaken to establish the geometric requirements for the above reaction.



(I) (II)

---

* IUPAC name: 2,3,4a*β*,9a*β*-tetramethyl-4(1*H*)-oxo-*cis*-4a,9a,-9,10-tetrahydro-1*β*-anthryl acetate (note that this numbering differs from that used throughout the paper).

0108-2701/87/061103-03$01.50