

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



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

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Hydrogen bonding, found in all the naphthoquinols studied, is present in this structure as O(2)- $H(2)\cdots O(1)$ interactions linking molecules along the *b* axis (Fig. 2): $O\cdots O = 2.885$ (5), $H\cdots O = 1.97$ Å, $O-H\cdots O = 160^{\circ}$.

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

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Abstract. $C_{20}H_{24}O_3$, $M_r = 312.41$, triclinic, $P\overline{1}$, a = 9.4624 (6), b = 9.7485 (7), c = 10.6743 (7) Å, $\alpha = 66.641$ (5), $\beta = 79.664$ (6), $\gamma = 70.336$ (6)°, V = 850.0 (1) Å³, Z = 2, $D_x = 1.220$ g cm⁻³, λ (Cu K α) = 1.5418 Å, $\mu = 5.963$ cm⁻¹, F(000) = 336, T = 295 K, R = 0.051 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.



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

Experimental. Crystal size $0.2 \times 0.2 \times 0.3$ mm, m.p. 405-406 K, Enraf-Nonius CAD-4 diffractometer, graphite-monochromatized Cu Ka radiation, lattice parameters from setting of 25 reflections with $33 \le \theta \le 47^{\circ}$, 3030 unique reflections with $\theta \le 75^{\circ}$, $h = -11 \rightarrow 11$, $k = -12 \rightarrow 12$, $l = 0 \rightarrow 13$; $\omega - 2\theta$ scan, ω scan width $(0.80+0.14\tan\theta)^\circ$, 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 MULTAN80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refined by full-matrix least squares minimizing $\sum w(|F_o| - |F_c|)^2$ using SHELX76 (Sheldrick, 1976). All H atoms were located in a difference synthesis and were refined isotropically. 304 parameters consisting of 141 positional parameters, 138 anisotropic temperature factors, 24 isotropic temperature factors and a scale factor. Convergence at R = 0.051, wR = 0.047 for 2391 observed reflections

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

| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | | $U_{eq} = \frac{1}{3} \sum_{i} \sum_{j} U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$ | | | | |
|---|--------------------------|--|------------------|--------------------|--------------------------|--|
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | | x | у | z | $U_{\rm eq}/U_{\rm iso}$ | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | O(1) | 9017 (2) | 2743 (2) | 9202 (2) | 65 | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | O(2) | 8044 (1) | 3202 (1) | 4318 (1) | 42 | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | O(3) | 8427 (2) | 1124 (2) | 3749 (2) | 83 | |
| $\begin{array}{cccccc} C(2) & 10093 (2) & 2592 (2) & 7095 (2) & 42 \\ C(21) & 11487 (3) & 2836 (4) & 7344 (3) & 64 \\ C(3) & 9871 (2) & 2516 (2) & 5911 (2) & 38 \\ C(31) & 11021 (3) & 2645 (3) & 4734 (2) & 56 \\ C(4) & 8478 (2) & 2224 (2) & 5715 (2) & 34 \\ C(41) & 8127 (2) & 2500 (2) & 3435 (2) & 47 \\ C(42) & 7823 (3) & 3674 (3) & 2018 (2) & 63 \\ C(44) & 7127 (2) & 2593 (2) & 6695 (2) & 35 \\ C(44) & 7127 (2) & 2593 (2) & 6695 (2) & 35 \\ C(44) & 6477 (2) & 4371 (2) & 6317 (2) & 46 \\ C(5) & 5917 (2) & 1922 (2) & 6593 (2) & 44 \\ C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(7) & 7411 (2) & -728 (2) & 8166 (2) & 43 \\ C(8) & 8396 (2) & 8 (2) & 8494 (2) & 44 \\ C(84) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(841) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 339 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1206 (3) & 241 (3) & 495 (3) & 78 (8) \\ H(41) & 586 (3) & 426 (3) & 529 (3) & 76 (7) \\ H(44) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(41) & 586 (3) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 779 (4) & 313 (5) & 146 (4) & 129 (12) \\ H(441) & 578 (3) & 456 (3) & 647 (2) & 65 (7) \\ H(441) & 598 (3) & 529 (3) & 559 (3) & 70 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(443) & 721 (3) & 488 (3) & 647 (2) & 65 (7) \\ H(441) & 598 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(421) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(421) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(4843) & 570 (3) & 154 (3) & 923 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(844) & 570 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) $ | C(1) | 8938 (2) | 2419 (2) | 8227 (2) | 42 | |
| $\begin{array}{cccccc} C(21) & 11487 (3) & 2836 (4) & 7344 (3) & 64 \\ C(3) & 9871 (2) & 2516 (2) & 5911 (2) & 38 \\ C(31) & 11021 (3) & 2645 (3) & 4734 (2) & 56 \\ C(4) & 8478 (2) & 2224 (2) & 5715 (2) & 34 \\ C(41) & 8127 (2) & 2500 (2) & 3435 (2) & 47 \\ C(42) & 7823 (3) & 3674 (3) & 2018 (2) & 63 \\ C(44) & 7127 (2) & 2593 (2) & 6695 (2) & 35 \\ C(441) & 6477 (2) & 4371 (2) & 6317 (2) & 46 \\ C(5) & 5917 (2) & 1922 (2) & 6593 (2) & 44 \\ C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(8) & 8396 (2) & 8 (2) & 8494 (2) & 44 \\ C(84) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(841) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(312) & 1113 (3) & 189 (4) & 436 (3) & 98 (10) \\ H(313) & 1072 (3) & 369 (4) & 400 (3) & 97 (9) \\ H(4) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(41) & 578 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(441) & 538 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(843) & 570 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(841) & 510 (3) & -2164 (3) & 723 (2) & 62 (6) \\ $ | C(2) | 10093 (2) | 2592 (2) | 7095 (2) | 42 | |
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| $\begin{array}{cccccc} C(4) & 8478 (2) & 2224 (2) & 5715 (2) & 34 \\ C(41) & 8127 (2) & 2500 (2) & 3435 (2) & 47 \\ C(42) & 7823 (3) & 3674 (3) & 2018 (2) & 63 \\ C(44) & 7127 (2) & 2593 (2) & 6695 (2) & 35 \\ C(44) & 7127 (2) & 2593 (2) & 6695 (2) & 35 \\ C(44) & 7127 (2) & 1922 (2) & 6593 (2) & 44 \\ C(5) & 5917 (2) & 164 (2) & 7238 (2) & 43 \\ C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(7) & 7411 (2) & -728 (2) & 8160 (2) & 43 \\ C(8) & 8396 (2) & 8 (2) & 8494 (2) & 44 \\ C(84) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(841) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6338 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(312) & 1113 (3) & 189 (4) & 436 (3) & 98 (10) \\ H(313) & 1072 (3) & 369 (4) & 400 (3) & 97 (9) \\ H(4) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (3) & 529 (3) & 80 (8) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(441) & 538 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(811) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(821) & 863 (4) & 151 (3) & 1014 (3) & 78 (8) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 590 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(843) & 570 (3) & 154 (3) & 923 (3) & 74 (7) \\ H(9) & 458 (3) & 7 (3) & 630 (3) & 83 (8) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(843) & 570 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(11) & 703 (3) & -418 (3) & 889 (3) & $ | C(31) | 11021 (3) | 2645 (3) | 4734 (2) | 56 | |
| $\begin{array}{ccccc} C(41) & 8127 (2) & 2500 (2) & 3435 (2) & 47 \\ C(42) & 7823 (3) & 3674 (3) & 2018 (2) & 63 \\ C(44) & 7127 (2) & 2593 (2) & 6695 (2) & 35 \\ C(441) & 6477 (2) & 4371 (2) & 6317 (2) & 46 \\ C(5) & 5917 (2) & 1922 (2) & 6593 (2) & 44 \\ C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(7) & 7411 (2) & -728 (2) & 8160 (2) & 43 \\ C(8) & 8396 (2) & 8 (2) & 8494 (2) & 44 \\ C(84) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(841) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -22349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1206 (3) & 241 (3) & 495 (3) & 78 (8) \\ H(312) & 1113 (3) & 189 (4) & 436 (3) & 98 (10) \\ H(313) & 1072 (3) & 369 (4) & 400 (3) & 97 (9) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 779 (4) & 313 (5) & 146 (4) & 129 (12) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 630 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(421) & 836 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(421) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(842) & 590 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 590 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & -418 (3) & 889 (3) & 87 (8) \\ H(10) & 510 (3) & -244 (3) & 723 (2) & 62 (6) \\ H(11) & 703 (3) & -418 (3) & 889 (3) & 87 (8) \\ H(10) & 510 (3) & -2164 (3) & 723 (2) & 62 (6) \\ H(11) & 703 (3) & -418 (3) &$ | C(4) | 8478 (2) | 2224 (2) | 5715 (2) | 34 | |
| $\begin{array}{ccccc} C(42) & 7823 (3) & 3674 (3) & 2018 (2) & 63 \\ C(44) & 7127 (2) & 2593 (2) & 6695 (2) & 35 \\ C(441) & 6477 (2) & 4371 (2) & 6177 (2) & 46 \\ C(5) & 5917 (2) & 1922 (2) & 6593 (2) & 44 \\ C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(7) & 7411 (2) & -728 (2) & 8160 (2) & 43 \\ C(8) & 8396 (2) & 8 (2) & 8494 (2) & 44 \\ C(84) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(841) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 66 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1072 (3) & 369 (4) & 400 (3) & 97 (9) \\ H(4) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 779 (4) & 313 (5) & 146 (4) & 129 (12) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(443) & 721 (3) & 488 (3) & 647 (2) & 65 (7) \\ H(441) & 558 (3) & 456 (3) & 529 (3) & 80 (8) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(443) & 721 (3) & 488 (3) & 647 (2) & 65 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(844) & 570 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(842) & 590 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(11) & 703 (3) & -418 (3) & 88 (93) & 87 (8) \\ \end{array}$ | C(41) | 8127 (2) | 2500 (2) | 3435 (2) | 47 | |
| $\begin{array}{ccccc} C(4.4) & 7127 (2) & 2593 (2) & 6695 (2) & 35 \\ C(4.41) & 6477 (2) & 4371 (2) & 6317 (2) & 46 \\ C(5) & 5917 (2) & 1922 (2) & 6593 (2) & 44 \\ C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(7) & 7411 (2) & -728 (2) & 8160 (2) & 43 \\ C(8) & 8396 (2) & 8 (2) & 8494 (2) & 44 \\ C(8.4) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(8.41) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1206 (3) & 241 (3) & 495 (3) & 78 (8) \\ H(312) & 1113 (3) & 189 (4) & 436 (3) & 98 (10) \\ H(4) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 779 (4) & 313 (5) & 129 (3) & 74 (7) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(313) & 712 (3) & 233 (3) & 559 (3) & 70 (7) \\ H(421) & 863 (4) & -23 (2) & 802 (2) & 48 (5) \\ H(421) & 863 (4) & -23 (2) & 802 (2) & 48 (5) \\ H(421) & 863 (4) & 131 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 771 (3) & 488 (3) & 647 (2) & 65 (7) \\ H(51) & 500 (2) & 241 (2) & 698 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(824) & 862 (2) & -54 (3) & 955 (3) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(823) & 570 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(841) & 10 & 703 (3) & -418 (3) & 889 (3) & 87 (8) \\ \end{array}$ | C(42) | 7823 (3) | 3674 (3) | 2018 (2) | 63 | |
| $\begin{array}{ccccc} C(4.41) & 6477 (2) & 4371 (2) & 6317 (2) & 46 \\ C(5) & 5917 (2) & 1922 (2) & 6593 (2) & 44 \\ C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(7) & 7411 (2) & -728 (2) & 8160 (2) & 43 \\ C(8) & 8396 (2) & 8 (2) & 8494 (2) & 44 \\ C(84) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(841) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -22349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1206 (3) & 241 (3) & 495 (3) & 78 (8) \\ H(312) & 1113 (3) & 189 (4) & 436 (3) & 98 (10) \\ H(4) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 779 (4) & 313 (5) & 146 (4) & 129 (12) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(441) & 558 (3) & 452 (3) & 659 (3) & 74 (7) \\ H(51) & 500 (2) & 241 (2) & 698 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(843) & 570 (3) & 154 (3) & 923 (3) & 74 (7) \\ H(9) & 458 (3) & 7 (3) & 630 (3) & 83 (8) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(811) & 703 (3) & -418 (3) & 889 (3) & 87 (8) \\ \end{array}$ | C(4A) | 7127 (2) | 2593 (2) | 6695 (2) | 35 | |
| $\begin{array}{ccccc} C(5) & 5917 (2) & 1922 (2) & 6593 (2) & 44 \\ C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(7) & 7411 (2) & -728 (2) & 8160 (2) & 43 \\ C(8) & 8396 (2) & 8 (2) & 8494 (2) & 44 \\ C(84) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(841) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1206 (3) & 241 (3) & 495 (3) & 78 (8) \\ H(421) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 779 (4) & 313 (5) & 146 (4) & 129 (12) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(443) & 721 (3) & 488 (3) & 647 (2) & 65 (7) \\ H(421) & 863 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(821) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(843) & 570 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(10) & 510 (3) & -248 (3) & 723 (2) & 62 (6) \\ H(10) & 510 (3) & -246 (3) & 723 (2) & 62 (6) \\ H(10) & 510 (3) & -246 (3) & 723 (2) & 62 (6) \\ H(11) & 703 (3) & -418 (3) & 889 (3) & 87 (8) \\ H(10) & 510 (3) & -418 (3) & 889 (3) & 87 (8) \\ H(10) & 510 (3) & -418 (3) & 889 (3)$ | C(4A1) | 6477 (2) | 4371 (2) | 6317 (2) | 46 | |
| $\begin{array}{ccccc} C(6) & 6279 (2) & 164 (2) & 7238 (2) & 43 \\ C(7) & 7411 (2) & -728 (2) & 8160 (2) & 43 \\ C(8) & 8396 (2) & 8 (2) & 8494 (2) & 44 \\ C(8A) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(8A1) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(11) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1206 (3) & 241 (3) & 495 (3) & 78 (8) \\ H(312) & 1113 (3) & 189 (4) & 436 (3) & 98 (10) \\ H(4) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 779 (4) & 313 (5) & 529 (3) & 80 (8) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(51) & 500 (2) & 241 (2) & 698 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(82) & 862 (2) & -54 (3) & 955 (3) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(843) & 570 (3) & 154 (3) & 923 (3) & 74 (7) \\ H(9) & 458 (3) & 7 (3) & 630 (3) & 83 (8) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(11) & 703 (3) & -418 (3) & 889 (3) & 87 (8) \\ \end{array}$ | C(5) | 5917 (2) | 1922 (2) | 6593 (2) | 44 | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(6) | 6279 (2) | 164 (2) | 7238 (2) | 43 | |
| $\begin{array}{ccccc} C(8) & 8396(2) & 8(2) & 8494(2) & 44 \\ C(84) & 7690(2) & 1789(2) & 8168(2) & 39 \\ C(841) & 6437(3) & 2044(3) & 9250(2) & 59 \\ C(9) & 5442(2) & -589(3) & 6932(2) & 55 \\ C(10) & 5720(3) & -2192(3) & 7532(3) & 64 \\ C(11) & 6838(3) & -3070(3) & 8440(3) & 66 \\ C(12) & 7673(3) & -2349(2) & 8755(2) & 54 \\ H(211) & 1225(5) & 187(5) & 775(5) & 146(15) \\ H(212) & 1189(4) & 359(5) & 661(4) & 120(11) \\ H(213) & 1133(4) & 331(5) & 802(4) & 134(13) \\ H(311) & 1206(3) & 241(3) & 495(3) & 78(8) \\ H(312) & 1113(3) & 189(4) & 436(3) & 98(10) \\ H(313) & 1072(3) & 369(4) & 400(3) & 97(9) \\ H(4) & 870(2) & 110(2) & 583(2) & 36(4) \\ H(421) & 863(4) & 413(4) & 171(4) & 114(11) \\ H(422) & 700(4) & 466(4) & 208(4) & 111(10) \\ H(423) & 779(4) & 313(5) & 146(4) & 129(12) \\ H(441) & 558(3) & 462(3) & 689(3) & 74(7) \\ H(442) & 620(3) & 496(3) & 529(3) & 80(8) \\ H(443) & 721(3) & 488(3) & 647(2) & 65(7) \\ H(421) & 862(2) & -23(2) & 802(2) & 48(5) \\ H(52) & 572(3) & 223(3) & 559(3) & 70(7) \\ H(81) & 938(2) & -23(2) & 802(2) & 48(5) \\ H(52) & 572(3) & 223(3) & 559(3) & 70(7) \\ H(81) & 938(2) & -23(2) & 802(2) & 48(5) \\ H(841) & 693(3) & 151(3) & 1014(3) & 78(8) \\ H(842) & 599(3) & 323(4) & 907(3) & 95(9) \\ H(843) & 570(3) & 154(3) & 723(2) & 62(6) \\ H(841) & 693(3) & 151(3) & 1014(3) & 78(8) \\ H(842) & 599(3) & 323(4) & 907(3) & 95(9) \\ H(842) & 599(3) & 323(4) & 907(3) & 95(9) \\ H(843) & 570(3) & 154(3) & 723(2) & 62(6) \\ H(841) & 693(3) & 151(3) & 1014(3) & 78(8) \\ H(842) & 599(3) & 323(4) & 907(3) & 95(9) \\ H(843) & 570(3) & 154(3) & 723(2) & 62(6) \\ H(841) & 693(3) & 151(3) & 73(2) & 62(6) \\ H(10) & 510(3) & -264(3) & 723(2) & 62(6) \\ H(11) & 703(3) & -418(3) & 889(3) & 87(8) \\ \end{array}$ | C(7) | 7411 (2) | -728 (2) | 8160 (2) | 43 | |
| $\begin{array}{cccccc} C(8.4) & 7690 (2) & 1789 (2) & 8168 (2) & 39 \\ C(8.4) & 6437 (3) & 2044 (3) & 9250 (2) & 59 \\ C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1206 (3) & 241 (3) & 495 (3) & 78 (8) \\ H(312) & 1113 (3) & 189 (4) & 436 (3) & 98 (10) \\ H(4) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 779 (4) & 313 (5) & 529 (3) & 80 (8) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(51) & 500 (2) & 241 (2) & 698 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(82) & 862 (2) & -54 (3) & 955 (3) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(843) & 570 (3) & 154 (3) & 923 (3) & 74 (7) \\ H(9) & 458 (3) & 7 (3) & 630 (3) & 83 (8) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(811) & 703 (3) & -418 (3) & 889 (3) & 87 (8) \\ \end{array}$ | C(8) | 8396 (2) | 8 (2) | 8494 (2) | 44 | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | C(8A) | 7690 (2) | 1789 (2) | 8168 (2) | 39 | |
| $\begin{array}{cccc} C(9) & 5442 (2) & -589 (3) & 6932 (2) & 55 \\ C(10) & 5720 (3) & -2192 (3) & 7532 (3) & 64 \\ C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1206 (3) & 241 (3) & 495 (3) & 78 (8) \\ H(312) & 1113 (3) & 189 (4) & 436 (3) & 98 (10) \\ H(313) & 1072 (3) & 369 (4) & 400 (3) & 97 (9) \\ H(4) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 779 (4) & 313 (5) & 146 (4) & 129 (12) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(443) & 721 (3) & 488 (3) & 647 (2) & 65 (7) \\ H(421) & 862 (2) & -53 (2) & 802 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 48 (5) \\ H(82) & 862 (2) & -54 (3) & 955 (3) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(843) & 570 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(842) & 599 (3) & 323 (4) & 907 (3) & 95 (9) \\ H(843) & 570 (3) & 154 (3) & 723 (2) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(11) & 703 (3) & -418 (3) & 889 (3) & 87 (8) \\ \end{array} $ | C(8A1) | 6437 (3) | 2044 (3) | 9250 (2) | 59 | |
| $\begin{array}{ccccccc} C(10) & 5720 & (3) & -2192 & (3) & 7532 & (3) & 64 \\ C(11) & 6838 & (3) & -3070 & (3) & 8440 & (3) & 66 \\ C(12) & 7673 & (3) & -22349 & (2) & 8755 & (2) & 54 \\ H(211) & 1225 & (5) & 187 & (5) & 775 & (5) & 146 & (15) \\ H(212) & 1189 & (4) & 359 & (5) & 661 & (4) & 120 & (11) \\ H(213) & 1133 & (4) & 331 & (5) & 802 & (4) & 134 & (13) \\ H(311) & 1206 & (3) & 241 & (3) & 495 & (3) & 78 & (8) \\ H(312) & 1113 & (3) & 189 & (4) & 436 & (3) & 98 & (10) \\ H(4) & 870 & (2) & 110 & (2) & 583 & (2) & 366 & (4) \\ H(421) & 863 & (4) & 413 & (4) & 171 & (4) & 114 & (11) \\ H(422) & 700 & (4) & 466 & (4) & 208 & (4) & 111 & (10) \\ H(423) & 779 & (4) & 313 & (5) & 146 & (4) & 129 & (12) \\ H(441) & 558 & (3) & 462 & (3) & 689 & (3) & 74 & (7) \\ H(442) & 620 & (3) & 496 & (3) & 529 & (3) & 80 & (8) \\ H(51) & 500 & (2) & 241 & (2) & 698 & (2) & 48 & (5) \\ H(52) & 572 & (3) & 223 & (3) & 559 & (3) & 70 & (7) \\ H(81) & 938 & (2) & -23 & (2) & 802 & (2) & 40 & (5) \\ H(82) & 862 & (2) & -54 & (3) & 955 & (3) & 62 & (6) \\ H(841) & 693 & (3) & 151 & (3) & 1014 & (3) & 78 & (8) \\ H(842) & 599 & (3) & 323 & (4) & 907 & (3) & 95 & (9) \\ H(843) & 570 & (3) & 154 & (3) & 223 & (3) & 83 & (8) \\ H(10) & 510 & (3) & -264 & (3) & 723 & (2) & 62 & (6) \\ H(11) & 703 & (3) & -418 & (3) & 889 & (3) & 87 & (8) \\ \end{array}$ | C(9) | 5442 (2) | -589 (3) | 6932 (2) | 55 | |
| $\begin{array}{cccccc} C(11) & 6838 (3) & -3070 (3) & 8440 (3) & 66 \\ C(12) & 7673 (3) & -2349 (2) & 8755 (2) & 54 \\ H(211) & 1225 (5) & 187 (5) & 775 (5) & 146 (15) \\ H(212) & 1189 (4) & 359 (5) & 661 (4) & 120 (11) \\ H(213) & 1133 (4) & 331 (5) & 802 (4) & 134 (13) \\ H(311) & 1206 (3) & 241 (3) & 495 (3) & 78 (8) \\ H(312) & 1113 (3) & 189 (4) & 436 (3) & 98 (10) \\ H(313) & 1072 (3) & 369 (4) & 400 (3) & 97 (9) \\ H(4) & 870 (2) & 110 (2) & 583 (2) & 36 (4) \\ H(421) & 863 (4) & 413 (4) & 171 (4) & 114 (11) \\ H(422) & 700 (4) & 466 (4) & 208 (4) & 111 (10) \\ H(423) & 779 (4) & 313 (5) & 146 (4) & 129 (12) \\ H(441) & 558 (3) & 462 (3) & 689 (3) & 74 (7) \\ H(442) & 620 (3) & 496 (3) & 529 (3) & 80 (8) \\ H(433) & 721 (3) & 488 (3) & 647 (2) & 65 (7) \\ H(51) & 500 (2) & 241 (2) & 698 (2) & 48 (5) \\ H(52) & 572 (3) & 223 (3) & 559 (3) & 70 (7) \\ H(81) & 938 (2) & -23 (2) & 802 (2) & 40 (5) \\ H(82) & 862 (2) & -54 (3) & 955 (3) & 62 (6) \\ H(841) & 693 (3) & 151 (3) & 1014 (3) & 78 (8) \\ H(843) & 570 (3) & 154 (3) & 923 (3) & 74 (7) \\ H(9) & 458 (3) & 7 (3) & 630 (3) & 83 (8) \\ H(10) & 510 (3) & -264 (3) & 723 (2) & 62 (6) \\ H(611) & 703 (3) & -418 (3) & 889 (3) & 87 (8) \\ \end{array}$ | C(10) | 5720 (3) | -2192 (3) | 7532 (3) | 64 | |
| $\begin{array}{ccccccc} C(12) & 7673 & (3) & -2349 & (2) & 8755 & (2) & 54 \\ H(211) & 1225 & (5) & 187 & (5) & 775 & (5) & 146 & (15) \\ H(212) & 1189 & (4) & 359 & (5) & 661 & (4) & 120 & (11) \\ H(213) & 1133 & (4) & 331 & (5) & 802 & (4) & 134 & (13) \\ H(311) & 1206 & (3) & 241 & (3) & 495 & (3) & 78 & (8) \\ H(312) & 1113 & (3) & 189 & (4) & 436 & (3) & 98 & (10) \\ H(313) & 1072 & (3) & 369 & (4) & 400 & (3) & 97 & (9) \\ H(4) & 870 & (2) & 110 & (2) & 583 & (2) & 36 & (4) \\ H(421) & 863 & (4) & 413 & (4) & 171 & (4) & 114 & (11) \\ H(422) & 770 & (4) & 466 & (4) & 208 & (4) & 111 & (10) \\ H(423) & 779 & (4) & 313 & (5) & 146 & (4) & 129 & (12) \\ H(441) & 558 & (3) & 462 & (3) & 689 & (3) & 74 & (7) \\ H(442) & 620 & (3) & 496 & (3) & 529 & (3) & 80 & (8) \\ H(443) & 721 & (3) & 488 & (3) & 647 & (2) & 65 & (7) \\ H(51) & 500 & (2) & 241 & (2) & 698 & (2) & 48 & (5) \\ H(52) & 572 & (3) & 223 & (3) & 559 & (3) & 70 & (7) \\ H(81) & 938 & (2) & -23 & (2) & 802 & (2) & 40 & (5) \\ H(821) & 862 & (2) & -54 & (3) & 955 & (3) & 62 & (6) \\ H(841) & 693 & (3) & 151 & (3) & 1014 & (3) & 78 & (8) \\ H(842) & 599 & (3) & 323 & (4) & 907 & (3) & 95 & (9) \\ H(843) & 570 & (3) & 154 & (3) & 923 & (3) & 74 & (7) \\ H(9) & 458 & (3) & 7 & (3) & 630 & (3) & 83 & (8) \\ H(10) & 510 & (3) & -264 & (3) & 723 & (2) & 62 & (6) \\ H(11) & 703 & (3) & -418 & (3) & 889 & (3) & 87 & (8) \\ \end{array}$ | C(11) | 6838 (3) | -3070 (3) | 8440 (3) | 66 | |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | C(12) | 7673 (3) | -2349 (2) | 8755 (2) | 54 | |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | H(211) | 1225 (5) | 187 (5) | 775 (5) | 146 (15) | |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | H(212) | 1189 (4) | 359 (5) | 661 (4) | 120 (11) | |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | H(213) | 1133 (4) | 331 (5) | 802 (4) | 134 (13) | |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | H(311) | 1206 (3) | 241 (3) | 495 (3) | 78 (8) | |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | H(312) | 1113 (3) | 189 (4) | 436 (3) | 98 (10) | |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | H(313) | 1072 (3) | 369 (4) | 400 (3) | 97 (9) | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | H(4) | 8/0(2) | 110 (2) | 583 (2) | 36 (4) | |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | H(421) | 803 (4) | 413 (4) | 1/1 (4) | 114 (11) | |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | H(422) | 700 (4) | 400 (4) | 208 (4) | 111 (10) | |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | H(423) | //9 (4) | 313 (5) | 146 (4) | 129 (12) | |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | $\Pi(4A1)$ | 556 (5) (20 (2) | 402 (3) | 689 (3) 630 (3) | 74 (7) | |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | $\Pi(4A2)$ $\Pi(AA2)$ | $\frac{020}{721}$ | 490 (3) | 529 (3) | 60 (6) 65 (7) | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | H(4A3) | 500 (2) | 400 (3) | 608 (2) | 49 (5) | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | H(57) | 572 (3) | 241 (2) | 550 (2) | 40 (3) | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | H(81) | 038 (2) | 223(3) | 802 (2) | 10(1) | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | H(81) | 862 (2) | -23(2) -54(3) | 055 (3) | 40 (J) 67 (6) | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | H(841) | 603 (3) | 151 (3) | 1014 (3) | 78 (8) | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | H(847) | 500 (3) | 323 (4) | 007 (3) | /0 (0) | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | H(843) | 570 (3) | 154 (3) | 907 (3) | 93 (9) 74 (7) | |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | H(9) | 458 (3) | 7 (3) | 630 (3) | 83 (2) | |
| H(11) 703 (3) -418 (3) 889 (3) 87 (8) | H(10) | 510 (3) | -264(3) | 723 (2) | 62 (6) | |
| | H(11) | 703 (3) | -418 (3) | 889 (3) | 87 (8) | |

-295 (3)

949 (3)

61 (6)

842 (3)

H(12)

for which $F \ge 3\sigma(F)$, where $\sigma^2(I)=S+2B+[0.04(S-B)]^2$, S = scan count, B = time-averaged background count. R = 0.072, wR = 0.052 for all data, $w = 1/\sigma^2(F)$, $(\Delta/\sigma)_{max} = 0.2$, $\pm 0.20 \text{ e} \text{ Å}^{-3}$ 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(4A)-C(8A) bond, so that the bridgehead methyl groups are staggered, as in the related compound $2,3,4a\beta,6,7,8a\beta$ -hexamethyl-4a,5,8,8a-tetrahydro-1-naphthoquin-4 β -yl acetate (III) (Ariel & Trotter, 1985). The degree of 'twist' is shown by the torsion angle C(4)-C(4A)-C(8A)-C(8), $-57.5(2)^{\circ}$, and C(4A1)-C(4A)-C(8A)-C(8A1), 60.8 (2)°. In (III) the corresponding values for the two angles are -58.9 (2) and 59.6 (2)°, respectively. Bond lengths and bond angles are not significantly different from those in (III), except for the increase in C(6)-C(7), 1.395 (3) vs. 1.326 (3) Å, resulting from the lower bond order. The $C(sp^3)$ - $C(sp^3)$ bond distances (Table 2) are in the range 1.529(3) - 1.554(3) Å, mean 1.541 Å.



Molecules of (I) crystallize with the conformation where the bulkier acetate substituent occupies the more sterically favoured pseudo-equatorial position, just like compound (III) (Ariel & Trotter, 1985). The consequence of this arrangement is the proximity of the β -enone carbon, C(3), to H(81) (2.85 Å). Furthermore, the angle between the C(3)...H(81) vector and its projection on the plane of C(3)=C(2) double bond [C(1),C(2),C(3),C(4)], τ , and the angle between the

C(3)...H(81) and the C(3)=C(2) vectors, Δ , are 49 and 74°, respectively. This geometry is highly favourable for H-abstraction by the β -enone C, which is observed

^{*} Lists of structure factors, anisotropic thermal parameters, and bond distances and angles involving hydrogen atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43702 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

| $\begin{array}{c} C(1)-O(1)\\ C(1)-C(2)\\ C(2)-C(3)\\ C(2)-C(3)\\ C(3)-C(4)\\ C(3)-C(4)\\ C(3)-C(4)\\ C(4)-O(2)\\ C(4)-O(2)\\ C(4)-O(2)\\ C(41)-O(3)\\ C(4)-C(4)\\ C(4)-C(5)\\ C(44)-C(5)\\ C(44)-C(5)\\ C(44)-C(441)\\ \end{array}$ | $\begin{array}{c} 1 \cdot 222 \ (3) \\ 1 \cdot 473 \ (3) \\ 1 \cdot 352 \ (3) \\ 1 \cdot 501 \ (4) \\ 1 \cdot 503 \ (3) \\ 1 \cdot 502 \ (3) \\ 1 \cdot 502 \ (3) \\ 1 \cdot 460 \ (2) \\ 1 \cdot 346 \ (3) \\ 1 \cdot 189 \ (3) \\ 1 \cdot 497 \ (3) \\ 1 \cdot 535 \ (3) \\ 1 \cdot 537 \ (2) \end{array}$ | $\begin{array}{c} C(5)-C(6)\\ C(6)-C(7)\\ C(7)-C(8)\\ C(8)-C(8A)\\ C(1)-C(8A)\\ C(4A)-C(8A)\\ C(8A)-C(8A)\\ C(6A)-C(8A)\\ C(6A)-C(9)\\ C(9)-C(10)\\ C(1)-C(11)\\ C(11)-C(12)\\ C(7)-C(12)\\ \end{array}$ | 1-511 (3) 1-395 (3) 1-510 (4) 1-552 (3) 1-523 (3) 1-554 (3) 1-396 (4) 1-383 (3) 1-376 (4) 1-375 (5) 1-400 (3) |
|--|--|---|--|
| $\begin{array}{l} \mathbb{C}(41) {=} O(2) {=} \mathbb{C}(4) \\ \mathbb{C}(2) {=} \mathbb{C}(1) {=} O(1) \\ \mathbb{C}(8A) {=} \mathbb{C}(1) {=} \mathbb{C}(2) \\ \mathbb{C}(21) {=} \mathbb{C}(2) {=} \mathbb{C}(1) \\ \mathbb{C}(3) {=} \mathbb{C}(2) {=} \mathbb{C}(1) \\ \mathbb{C}(3) {=} \mathbb{C}(2) {=} \mathbb{C}(2) \\ \mathbb{C}(3) {=} \mathbb{C}(2) \\ \mathbb{C}(4) {=} \mathbb{C}(3) {=} \mathbb{C}(2) \\ \mathbb{C}(4) {=} \mathbb{C}(3) {=} \mathbb{C}(2) \\ \mathbb{C}(4A) {=} \mathbb{C}(4A) {=} \mathbb{C}(3) \\ \mathbb{C}(4A) {=} \mathbb{C}(4A) {=} \mathbb{C}(3) \\ \mathbb{C}(3A) {=} \mathbb{C}(4A) {=} \mathbb{C}(4A) \\ \mathbb{C}(5) {=} \mathbb{C}(4A) {=} \mathbb{C}(4A) \\ \mathbb{C}(5A) {=} \mathbb{C}(4A) {=} \mathbb{C}(4) \\ \mathbb{C}(5A) {=} \mathbb{C}(4A) {=} \mathbb{C}(4) \\ \mathbb{C}(4A) {=} \mathbb{C}(4A) \\ \mathbb{C}(4A) = \mathbb{C}(4A) \\ \mathbb{C}(4A) {=} \mathbb{C}(4A) \\ \mathbb{C}(4A) = \mathbb{C}(4A) \\ \mathbb{C}(4A) \\ \mathbb{C}(4A) = \mathbb{C}(4A) \\ \mathbb{C}(4A) \\ \mathbb{C}(4A) = \mathbb{C}(4A) \\ \mathbb{C}(4A) \\ \mathbb{C}(4A) \\ \mathbb{C}(4A) = \mathbb{C}(4A) \\ \mathbb$ | $\begin{array}{c} 118.5 (1) \\ 119.9 (2) \\ 121.4 (2) \\ 118.7 (2) \\ 118.7 (2) \\ 119.9 (2) \\ 123.4 (2) \\ 122.4 (2) \\ 122.4 (2) \\ 122.4 (2) \\ 121.8 (2) \\ 115.7 (1) \\ 108.3 (1) \\ 107.4 (1) \\ 109.9 (2) \\ 109.6 (2) \\ 110.9 (2) \\ 109.6 (2) \\ 109.6 (1) \\ 111.1 (2) \end{array}$ | $\begin{array}{c} C(42)-C(41)-O(3)\\ O(3)-C(41)-O(2)\\ C(44)-C(5)-C(6)\\ C(7)-C(6)-C(5)\\ C(9)-C(6)-C(5)\\ C(9)-C(6)-C(7)\\ C(8)-C(7)-C(6)\\ C(12)-C(7)-C(6)\\ C(12)-C(7)-C(8)\\ C(84)-C(84)-C(1)\\ C(84)-C(84)-C(1)\\ C(8)-C(84)-C(44)\\ C(841)-C(84)-C(1)\\ C(8)-C(84)-C(1)\\ C(841)-C(84)-C(1)\\ C(841)-C(84)-C(1)\\ C(841)-C(84)-C(1)\\ C(841)-C(84)-C(1)\\ C(841)-C(84)-C(1)\\ C(841)-C(84)-C(1)\\ C(1)-C(9)-C(6)\\ C(11)-C(10)-C(9)\\ C(11)-C(10)\\ $ | $\begin{array}{c} 125\cdot1\ (2)\\ 123\cdot8\ (2)\\ 115\cdot1\ (2)\\ 121\cdot6\ (2)\\ 119\cdot5\ (2)\\ 119\cdot5\ (2)\\ 119\cdot5\ (2)\\ 119\cdot5\ (2)\\ 119\cdot2\ (2)\\ 110\cdot2\ (2)\\ 106\cdot9\ (2)\\ 110\cdot2\ (2)\\ 106\cdot9\ (2)\\ 110\cdot2\ (2)\\ 106\cdot9\ (2)\\ 110\cdot2\ (2)\\ 108\cdot9\ (2)\\ 120\cdot9\ (2)\\ 120\cdot9\ (2)\\ 120\cdot1\ (3)\\ 119\cdot8\ (2)\\ 121\cdot1\ (2)\ (2)\ (2)\ (2)\ (2)\ (2)\ (2)\ (2)$ |
| $\begin{array}{l} C(41)-O(2)-C(4)-C(3)\\ C(4)-O(2)-C(4)-C(4)\\ C(4)-O(2)-C(4)-C(4)\\ C(4)-O(2)-C(4)-C(4)\\ C(4)-O(2)-C(4)-C(4)\\ C(4)-O(2)-C(4)-C(2)-C(2)\\ C(8A)-C(1)-C(2)-C(2)\\ C(8A)-C(1)-C(2)-C(3)\\ O(1)-C(1)-C(8A)-C(4A\\ O(1)-C(1)-C(8A)-C(4A\\ C(2)-C(1)-C(8A)-C(4A\\ C(2)-C(1)-C(8A)-C(4A\\ C(2)-C(1)-C(8A)-C(4A\\ C(2)-C(3)-C(4)-C(4A\\ C(3))-C(3)-C(4)-C(4A\\ O(2)-C(4)-C(4A)-C(5)\\ O(2)-C(4)-C(4)-C(4)\\ O(2)-C(4)-C(4)-C(4)\\ O(2)-C(4)-C(4)-C(4)\\ O(2)-C(4)-C(4)\\ O(2)-C(4)-C(4)\\ O(2)-C(4)$ |)) () (1)) (1)) (1) | $\begin{array}{c} 113 \cdot 5 \ (2) \\ -121 \cdot 6 \ (2) \\ 5 \cdot 9 \ (3) \\ -173 \cdot 1 \ (2) \\ 12 \cdot 6 \ (3) \\ -165 \cdot 6 \ (2) \\ 14 \cdot 0 \ (3) \\ 138 \cdot 3 \ (2) \\ -103 \cdot 7 \ (2) \\ 14 \cdot 5 \ (3) \\ -43 \cdot 5 \ (2) \\ 74 \cdot 5 \ (2) \\ -167 \cdot 4 \ (2) \\ -1-3 \ (3) \\ 141 \cdot 3 \ (2) \\ 20 \cdot 6 \ (3) \\ -41 \cdot 3 \ (2) \\ 20 \cdot 6 \ (3) \\ -41 \cdot 3 \ (2) \\ -161 \cdot 9 \ (2) \\ -48 \cdot 5 \ (2) \\ 71 \cdot 9 \ (2) \\ -169 \cdot 4 \ (1) \end{array}$ | |
| $\begin{array}{c} C(3)-C(4)-C(4A)-C(4A)-C(4A)\\ C(3)-C(4)-C(4A)-C(5)\\ C(3)-C(4)-C(4A)-C(5)-C(6)\\ C(4)-C(4)-C(4)-C(5)-C(6)\\ C(4)-C(4)-C(8)-C(6)\\ C(4)-C(4)-C(8)-C(6)\\ C(4)-C(4)-C(8)-C(6)\\ C(4)-C(4)-C(8)-C(8)-C(6)\\ C(4)-C(4)-C(8)-C(8)-C(6)\\ C(4)-C(4)-C(8)-C(8)-C(6)\\ C(4)-C(4)-C(8)-C(8)-C(6)\\ C(4)-C(4)-C(8)-C(6)\\ C(4)-C(4)-C(8)-C(6)\\ C(4)-C(4)-C(8)-C(6)\\ C(5)-C(4)-C(8)-C(6)\\ C(5)-C(4)-C(8)-C(6)\\ C(7)-C(8)-C(8)-C(8)-C(8)\\ C(7)-C(8)-C(8)-C(4)-C(8)-C(4)\\ C(7)-C(8)-C(8)-C(8)-C(4)\\ C(7)-C(8)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(7)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(7)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)\\ C(8)-C(8)-C(8)\\ C(8)-C(8)\\ C(8)-C(8)-C(8)\\ C(8)-C(8)\\ C(8)-C(8)\\ C(8)-C(8)\\ C(8)-C(8)\\ C(8)-C(8)\\ C(8)\\ C(8)-C(8)\\ C(8)\\ C$ | (6) (6) (1) (3) (4) (1) (1) (1) (1) (1) (1) (1) (1 | $\begin{array}{c} 71 \cdot 6 \ (2) \\ -168 \cdot 0 \ (2) \\ -49 \cdot 3 \ (2) \\ 72 \cdot 8 \ (2) \\ -166 \cdot 7 \ (2) \\ -44 \cdot 8 \ (2) \\ 58 \cdot 8 \ (2) \\ -57 \cdot 5 \ (2) \\ -178 \cdot 9 \ (2) \\ -61 \cdot 5 \ (2) \\ -177 \cdot 8 \ (2) \\ 60 \cdot 8 \ (2) \\ 177 \cdot 5 \ (2) \\ 61 \cdot 2 \ (2) \\ 161 \cdot 2 \ (2) \\ -60 \cdot 2 \ (2) \\ 16 \cdot 4 \ (3) \\ -165 \cdot 1 \ (2) \\ 20 \cdot 9 \ (3) \\ -161 \cdot 2 \ (2) \ $ | |





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

in the solid state and solution photolysis, followed by C(2)-C(8) bonding, $C(2)\cdots C(8) = 3.168$ (3) Å, to generate compound (II). The corresponding values for the C(3)...H(81) distance, τ , and Δ for compound (III), are 2.84 Å, 50, and 74°, respectively, allowing the H-abstraction by the β -enone C photolysis to occur in the solid state (Ariel & Trotter, 1985).

The distance between the carbonyl oxygen, O(1), and the β -hydrogen, H(82), is 3.21 Å, larger than the 2.7 Å van der Waals O...H contact; thus, the photochemical reaction pathway for β -hydrogen abstraction from C(8) by O(1) is not feasible. O(1) is 2.50 Å away from another β -hydrogen, H(8A1), and the other relevant geometric parameters for this 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 $\tau = 8^{\circ}$, $\Delta = 81^{\circ}$. Thus there is an almost perfect alignment of the β -H with the non-bonding orbital of O(1). However, no such product has been observed.

Intermolecular distances correspond to normal van der Waals interactions.

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