1976) and its D-*erythro* isomer (Ružić-Toroš & Lazarini, 1978), 2-acetamido-2,3-dideoxy-5,6-*O*-isopropylidene-D-*threo*-hex-2-enono-1,4-lactone (Ružić-Toroš & Leban, 1978), and L-ascorbic acid (Hvoslef, 1968).

Molecules are connected by hydrogen bonds between acetamido and carbonyl groups, N—H(N)···O(1), 3·000 (4) Å, forming infinite chains along **b**. The angle N—H(N)···O(1) is 171 (2)°.

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Structure of (*E*)-2-Ethynyl-2-methoxy-5-phenyladamantane*†

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Abstract. $C_{19}H_{22}O$, orthorhombic, $Pc2_1n$, a = 6·972 (2), b = 20·214 (7), c = 21·025 (6) Å, V = 2961 Å^3, Z = 8, ρ_o = 1·199 g cm^{-3}. R = 0·057 for 2065 observed reflections measured on a diffractometer using Cu $K\alpha$ radiation. The two chemically independent molecules in the asymmetric unit are arranged around a pseudo center of symmetry and the pairs thus generated pack in the structure using the symmetry of the space group. The OCH_3 group is in the *anti* configuration with respect to the phenyl group.

Introduction. This report is part of our systematic investigation into bridgehead phenyl-substituted adamantanes to determine their configurations and to study reaction mechanisms involving these compounds. Thus, in a methanolysis of (*E*)- and (*Z*)-2-chloro-2-ethynyl-5-phenyladamantanes,§ $C_{10}H_{13}.C_6H_5.(C{\equiv}CH).Cl$, these two isomers both produce the same mixture of 2-ethynyl-2-methoxy-5-phenyladamantanes. Regardless of the configuration of the starting isomer, it was observed that the product is a mixture of 3:1 in favor of one of the configurations, (*Z*) (le Noble, Chiou & Okaya, 1978). It was then postulated that the two reactions go through a common intermediate, and this is attacked preferentially from one side by CH_3OH because of a remote directing effect of the phenyl group in the 5-position. In view of this remarkable preference in the collapse of the intermediate, it seemed desirable to confirm the

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* IUPAC name: (*E*)-2-ethynyl-2-methoxy-5-phenyltricyclo[3.3.1.1^{3,7}]decane.

† Crystallographic Studies on Adamantanes. IV.

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§ The configurations of these isomers were unambiguously determined by crystallographic methods (Okaya, Lin, Chiou & le Noble, 1980).

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Table 1. *Fractional atomic coordinates and isotropic thermal parameters*

For non-H atoms $B_{eq} = \frac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j$.

	x	*y*	*z*	B_{eq}/B (Å^2)
Molecule *A*				
O(1*A*)	0·1539 (3)	0·1770 (1)	0·1961 (1)	4·45 (2)
C(1*A*)	0·2676 (5)	0·1406 (2)	0·0957 (2)	3·93 (2)
C(2*A*)	0·2926 (5)	0·1914 (2)	0·1487 (2)	3·63 (2)
C(3*A*)	0·2667 (5)	0·2607 (2)	0·1192 (3)	3·86 (2)
C(4*A*)	0·4230 (5)	0·2714 (2)	0·0665 (2)	4·09 (3)
C(5*A*)	0·3981 (5)	0·2207	0·1038 (2)	3·60 (2)
C(6*A*)	0·1953 (5)	0·2267 (2)	−0·1036 (2)	4·12 (3)
C(7*A*)	0·0480 (5)	0·2146 (2)	0·0383 (2)	4·74 (4)
C(8*A*)	0·0690 (5)	0·1463 (2)	0·0670 (2)	4·73 (3)
C(9*A*)	0·0665 (5)	0·2660 (2)	0·0900 (2)	4·92 (3)
C(10*A*)	0·4204 (5)	0·1511 (2)	0·0432 (2)	4·14 (3)
C(1*pA*)	0·5462 (5)	0·2316 (2)	−0·0398 (1)	3·43 (2)
C(2*pA*)	0·6044 (6)	0·2950 (2)	−0·0554 (2)	5·34 (3)
C(3*pA*)	0·7377 (7)	0·3061 (2)	−0·1038 (2)	6·23 (4)
C(4*pA*)	0·8097 (5)	0·2535 (2)	−0·1394 (2)	5·08 (3)
C(5*pA*)	0·7527 (6)	0·1924 (2)	−0·1230 (2)	5·64 (3)
C(6*pA*)	0·6221 (5)	0·1794 (2)	−0·0742 (2)	5·22 (3)
C(1*eA*)	0·4862 (5)	0·1848 (2)	0·1774 (2)	4·69 (3)
C(2*eA*)	0·6391 (6)	0·1784 (3)	0·1981 (2)	6·61 (4)
C(1*mA*)	0·1544 (6)	0·2181 (2)	0·2506 (2)	5·76 (3)
H(1*A*)	0·281 (5)	0·092 (2)	0·119 (1)	4·3 (7)
H(3*A*)	0·271 (5)	0·287 (2)	0·156 (1)	3·7 (7)
H(4*A*)	0·414 (4)	0·322 (2)	0·054 (2)	5·0 (8)
H(4*A*′)	0·547 (4)	0·275 (2)	0·090 (1)	3·9 (7)
H(6*A*)	0·178 (4)	0·193 (2)	−0·046 (2)	4·9 (8)
H(6*A*′)	0·175 (5)	0·272 (2)	−0·035 (2)	5·7 (9)
H(7*A*)	−0·070 (6)	0·213 (3)	0·012 (2)	5·7 (13)
H(8*A*)	0·079 (5)	0·099 (2)	0·036 (2)	6·2 (10)
H(8*A*′)	0·944 (4)	0·139 (2)	0·103 (2)	4·4 (8)
H(9*A*)	−0·044 (4)	0·264 (2)	0·125 (2)	4·8 (8)
H(9*A*′)	0·069 (4)	0·314 (2)	0·078 (2)	7·6 (0)
H(10*A*)	0·423 (5)	0·121 (2)	0·006 (2)	7·4 (11)
H(10*A*′)	0·544 (5)	0·139 (2)	0·059 (2)	6·3 (9)
H(2*pA*)	0·571 (4)	0·336 (2)	−0·026 (2)	4·1 (7)
H(3*pA*)	0·830 (6)	0·348 (3)	−0·096 (2)	4·0 (12)
H(4*pA*)	0·886 (6)	0·268 (3)	−0·179 (2)	12·4 (15)
H(5*pA*)	0·800 (5)	0·160 (2)	−0·148 (2)	7·4 (10)
H(6*pA*)	0·548 (5)	0·134 (2)	−0·069 (2)	7·9 (9)
H(2*eA*)	0·778 (9)	0·174 (3)	0·203 (3)	11·0 (16)
H(1*mA*)	0·107 (5)	0·269 (2)	0·239 (2)	6·5 (10)
H(2*mA*)	0·061 (5)	0·190 (2)	0·286 (2)	8·2 (9)
H(3*mA*)	0·286 (9)	0·242 (3)	0·266 (3)	4·0 (19)
Molecule *B*				
O(1*B*)	0·8472 (3)	0·5008 (1)	0·0463 (1)	4·60 (2)
C(1*B*)	0·7223 (5)	0·5426 (2)	0·1441 (2)	4·37 (3)
C(2*B*)	0·7091 (5)	0·4862 (1)	0·0954 (1)	3·96 (3)
C(3*B*)	0·7498 (5)	0·4210 (2)	0·1296 (2)	4·00 (2)
C(4*B*)	0·5980 (5)	0·4102 (2)	0·1817 (2)	3·79 (3)
C(5*B*)	0·6037 (4)	0·4658 (2)	0·2320 (1)	3·39 (2)
C(6*B*)	0·8122 (5)	0·4676 (2)	0·2602 (2)	4·48 (3)
C(7*B*)	0·9615 (5)	0·4780 (2)	0·2086 (2)	4·58 (3)
C(8*B*)	0·9240 (5)	0·5434 (2)	0·1743 (2)	5·02 (3)
C(9*B*)	0·9483 (5)	0·4221 (2)	0·1598 (2)	4·83 (3)
C(10*B*)	0·5716 (5)	0·5316 (2)	0·1970 (2)	4·08 (3)
C(1*pB*)	0·4613 (4)	0·4557 (2)	0·2836 (1)	3·61 (2)
C(2*pB*)	0·3771 (5)	0·3940 (2)	0·2964 (2)	4·89 (3)
C(3*pB*)	0·2452 (6)	0·3856 (2)	0·3454 (2)	5·60 (3)
C(4*pB*)	0·1880 (6)	0·4384 (2)	0·3808 (2)	5·27 (3)
C(5*pB*)	0·2677 (6)	0·4997 (2)	0·3703 (2)	5·66 (3)
C(6*pB*)	0·4028 (5)	0·5075 (2)	0·3226 (2)	4·45 (2)
C(1*eB*)	0·5144 (5)	0·4868 (2)	0·0664 (1)	4·21 (3)
C(2*eB*)	0·3570 (6)	0·4882 (3)	0·0450 (2)	6·36 (4)
C(1*mB*)	0·8421 (6)	0·4586 (3)	−0·0076 (2)	6·04 (4)
H(1*B*)	0·694 (5)	0·587 (2)	0·127 (2)	4·5 (8)
H(3*B*)	0·753 (5)	0·380 (1)	0·101 (1)	4·0 (7)
H(4*B*)	0·615 (4)	0·369 (1)	0·204 (1)	2·8 (6)
H(4*B*′)	0·479 (8)	0·409 (3)	0·164 (3)	10·7 (16)

Table 1 (*cont.*)

	x	*y*	*z*	*B* (Å^2)
H(6*B*)	0·807 (5)	0·507 (2)	0·298 (2)	6·5 (10)
H(6*B*′)	0·847 (5)	0·425 (3)	0·286 (3)	7·9 (12)
H(7*B*)	1·083 (5)	0·481 (2)	0·226 (2)	6·2 (10)
H(8*B*)	0·924 (6)	0·575 (3)	0·206 (3)	8·4 (15)
H(8*B*′)	1·030 (6)	0·550 (2)	0·145 (2)	6·5 (9)
H(9*B*)	1·069 (6)	0·437 (3)	0·131 (3)	9·4 (14)
H(9*B*′)	0·973 (9)	0·374 (4)	0·183 (3)	12·3 (20)
H(10*B*)	0·574 (8)	0·565 (4)	0·231 (3)	4·1 (0)
H(10*B*′)	0·436 (8)	0·529 (4)	0·180 (4)	5·1 (0)
H(2*pB*)	0·428 (9)	0·358 (4)	0·270 (3)	4·0 (20)
H(3*pB*)	0·246 (6)	0·330 (2)	0·361 (2)	5·0 (9)
H(4*pB*)	0·066 (5)	0·427 (2)	0·419 (2)	5·3 (9)
H(5*pB*)	0·230 (9)	0·530 (3)	0·400 (2)	12·7 (16)
H(6*pB*)	0·450 (6)	0·555 (3)	0·310 (2)	8·3 (13)
H(2*eB*)	0·219 (7)	0·490 (3)	0·018 (2)	11·2 (12)
H(1*mB*)	0·827 (7)	0·406 (3)	0·003 (2)	12·0 (18)
H(2*mB*)	0·937 (6)	0·463 (2)	−0·039 (2)	9·9 (13)
H(3*mB*)	0·741 (8)	0·471 (3)	−0·031 (2)	11·0 (14)

molecular configurations of the products by means of crystallographic studies.

The present compound, $C_{10}H_{13}.C_6H_5.(C\equiv CH).OCH_3$, has been chemically assigned the configuration *E*. The observed systematic absences lead to the choice of space groups as *Pcmn* or $Pc2_1n$. The diffractometer data were collected on an Enraf–Nonius CAD-4A diffractometer, which is a part of a real-time in-house crystallographic system built around a resource-sharing PDP-11/45 computer (Okaya, 1978). The θ–2θ scan method was used for reflections below 65° in θ using Cu $K\alpha$ radiation. In all, 2815 asymmetric reflections were collected out of which 2065 were classified to be observed by means of the 3σ criterion.

Although a statistical treatment of the magnitudes of *E* factors favors strongly the presence of centers of symmetry, repeated attempts in solving the structure by *MULTAN* (Germain, Main & Woolfson, 1971) in *Pcmn* led to no satisfactory solution. It is also rather unusual for organic molecules of this type to form a structure with mirror symmetry as required by this space group. When the polar $Pc2_1n$ space group was employed, the direct method quickly gave a reasonable starting structure as a solution; it was then refined by a full-matrix least-squares program using the *Enraf–Nonius Structure Determination Package* on the in-house PDP 11/45 computer (Frenz, 1978). The function minimized was $\sum w(F_o^2 - kF_c^2)^2$ with $w^{-1} = [\sigma_{c.s.}F_o^2 + (0{\cdot}03F_o^2)^2]$, where $\sigma_{c.s.}$ is the deviation depending on the counting statistics. All the H atoms have been located in difference Fourier maps and refined with isotropic temperature factors. The final disagreement factor, *R*, is 0·057. The atomic scattering factors used in the calculations are those derived by Cromer & Waber (1974). The atomic parameters thus determined are tabulated in Table 1.* The two independent molecules required by the space-group symmetry are arbitrarily labeled *A* and *B*.

Discussion. The bond distances and angles were calculated from the atomic coordinates in Table 1; these are tabulated in Tables 2 and 3. The numbering of the atoms used in the following discussion is shown in Fig. 1. The compound was determined to possess the *E* configuration as chemically assigned.

An interesting feature of the crystal structure is that the two structurally independent molecules in the asymmetric unit are arranged around a pseudo non-crystallographic center of symmetry at $x \simeq 0{\cdot}0$ and $z \simeq 0{\cdot}125$ ($=\frac{1}{8}$); the y parameter (= 0·342 with respect to the origin on the *b* axis used in Table 1) has only relative significance because of the polar nature of the *b* axis. As shown in Table 1, observed deviation from this pseudo-centrosymmetry is relatively small (maximum 0·3 Å). It should be noted that no linear transformation of the cell results in *Pcmn* or any other space group with higher symmetry elements. The centrosymmetric pairs thus formed are arranged in the structure by satisfying the requirements of the polar space group $Pc2_1n$. An *ORTEP* (Johnson, 1965) drawing of the pair is given in Fig. 2.

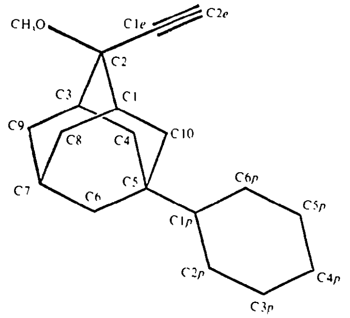

Fig. 1. The numbering of atoms used in the *Discussion*.

It is also obvious from the above structure that the two crystallographically different molecules exhibit almost identical orientations of the phenyl group with respect to the approximate mirror plane [C(2)—C(5)—C(6)—C(7)] through the adamantane moiety. The dihedral angles between these mirror and phenyl group planes are found to be 87 and 80° for *A* and *B* respectively. This situation is different from that found in two similar crystallographically independent molecules of (*Z*)-2-ethynyl-5-phenyl-2-adamantanol,

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36639 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances in* Å

	Molecule *A*	Molecule *B*		Molecule *A*	Molecule *B*
C(1)—C(2)	1·526 (4)	1·536 (4)	C(6)—C(7)	1·518 (5)	1·517 (4)
C(1)—C(8)	1·514 (5)	1·541 (4)	C(7)—C(8)	1·513 (5)	1·528 (5)
C(1)—C(10)	1·548 (4)	1·545 (4)	C(7)—C(9)	1·510 (5)	1·531 (5)
C(2)—C(3)	1·542 (5)	1·527 (5)	C(1*p*)—C(2*p*)	1·383 (4)	1·404 (5)
C(2)—C(1*e*)	1·484 (4)	1·487 (4)	C(1*p*)—C(6*p*)	1·385 (4)	1·392 (4)
C(2)—O(1)	1·419 (3)	1·441 (3)	C(2*p*)—C(3*p*)	1·396 (4)	1·391 (4)
C(3)—C(4)	1·568 (4)	1·539 (4)	C(3*p*)—C(4*p*)	1·393 (6)	1·360 (6)
C(3)—C(9)	1·528 (5)	1·522 (5)	C(4*p*)—C(5*p*)	1·342 (6)	1·376 (6)
C(4)—C(5)	1·520 (4)	1·543 (4)	C(5*p*)—C(6*p*)	1·396 (5)	1·385 (4)
C(5)—C(6)	1·531 (4)	1·570 (4)	C(1*e*)—C(2*e*)	1·158 (4)	1·186 (4)
C(5)—C(10)	1·545 (4)	1·537 (4)	O(1)—C(1*m*)	1·415 (4)	1·415 (4)
C(5)—C(1*p*)	1·545 (4)	1·484 (4)			

Table 3. *Bond angles in degrees*

	Molecule *A*	Molecule *B*		Molecule *A*	Molecule *B*		Molecule *A*	Molecule *B*
C(2)—C(1)—C(8)	110·1 (3)	109·7 (3)	C(3)—C(4)—C(5)	110·1 (2)	111·5 (2)	C(3) C(9)—C(7)	108·5 (3)	110·2 (2)
C(2)—C(1)—C(10)	110·3 (3)	109·5 (2)	C(4)—C(5)—C(6)	109·1 (2)	107·5 (2)	C(1)—C(10)—C(5)	109·9 (2)	111·6 (2)
C(8)—C(1)—C(10)	109·6 (2)	109·0 (3)	C(4)—C(5)—C(10)	108·1 (2)	107·4 (2)	C(5)—C(1*p*)—C(2*p*)	120·1 (2)	122·8 (3)
C(1)—C(2)—C(3)	107·7 (2)	108·3 (2)	C(4)—C(5)—C(1*p*)	111·2 (2)	112·6 (2)	C(5)—C(1*p*)—C(6*p*)	121·9 (3)	121·6 (3)
C(1)—C(2)—C(1*e*)	109·0 (3)	108·8 (3)	C(6)—C(5)—C(10)	108·4 (2)	107·2 (2)	C(2*p*)—C(1*p*)—C(6*p*)	118·0 (3)	115·7 (3)
C(1)—C(2)—O(1)	107·3 (2)	106·6 (3)	C(6)—C(5)—C(1*p*)	109·4 (2)	110·3 (2)	C(1*p*)—C(2*p*)—C(3*p*)	121·2 (3)	121·8 (3)
C(3)—C(2)—C(1*e*)	110·6 (3)	111·7 (3)	C(10)—C(5)—C(1*p*)	110·8 (2)	111·9 (2)	C(2*p*)—C(3*p*)—C(4*p*)	120·6 (4)	120·2 (4)
C(3)—C(2)—O(1)	112·9 (3)	112·9 (3)	C(5)—C(6)—C(7)	109·9 (2)	111·6 (2)	C(3*p*)—C(4*p*)—C(5*p*)	117·2 (4)	120·2 (3)
C(1*e*)—C(2)—O(1)	108·4 (2)	108·3 (2)	C(6)—C(7)—C(8)	111·6 (3)	109·9 (3)	C(4*p*)—C(5*p*)—C(6*p*)	123·7 (4)	119·6 (4)
C(2)—C(3)—C(4)	109·2 (3)	109·3 (3)	C(6)—C(7)—C(9)	110·4 (3)	109·6 (3)	C(1*p*)—C(6*p*)—C(5*p*)	119·3 (3)	122·7 (4)
C(2)—C(3)—C(9)	109·4 (3)	110·7 (3)	C(8)—C(7)—C(9)	109·4 (3)	108·1 (3)	C(2)—C(1*e*)—C(2*e*)	177·7 (4)	178·0 (3)
C(4)—C(3)—C(9)	109·9 (3)	109·2 (3)	C(1)—C(8)—C(7)	108·4 (3)	109·9 (2)	C(2)—O(1)—C(1*m*)	116·5 (2)	115·7 (2)

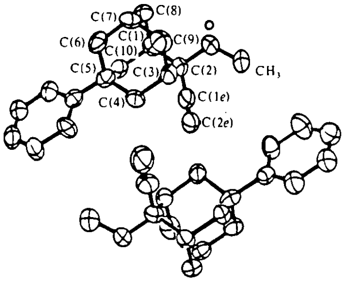

Fig. 2. An *ORTEP* drawing of a pseudo-centrosymmetric pair.

$C_{10}H_{13}.C_6H_5.(C{\equiv}CH).OH$, (Okaya, Chiou & le Noble, 1979). In this molecule the dihedral angles are quite different from each other (10·5 and 44·5°).

The observed bond distances and angles are all normal for this type of compound. The C(2*p*)—C(1*p*)—C(6*p*) angles of 115·7 (3) and 118·0 (3)° are smaller than the normal angles of 120°. The appearance of smaller angles is common to all the phenyladamantanes studied by us (le Noble, Chiou, Małuszyńska & Okaya, 1977), and the structure serves as another example of the non-bonded steric-hindrance effect as discussed by Domenicano, Vaciago & Coulson (1975). The steric effect around the methoxy bond is such that it is almost parallel to the O(1)—C(2)—C(1)—C(10) plane.

The molecules are arranged in the structure by the usual van der Waals interactions. No unusual intermolecular contacts were observed.

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Structure of 2-Ethynyl-2-adamantanol*†

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Abstract. $C_{12}H_{16}O$, monoclinic, $P2_1/c$, $a = 6{\cdot}820$ (2), $b = 22{\cdot}644$ (3), $c = 12{\cdot}708$ (2) Å, $\beta = 94{\cdot}5$ (2)°, $V = 1956{\cdot}5$ Å^3, $Z = 8$, $\rho_o \simeq \rho_c = 1{\cdot}19$ g cm^{-3}. $R = 5{\cdot}0$% for 2200 observed reflections measured on a diffractometer using Cu $K\alpha$ radiation. The two crystallographically independent molecules in the asymmetric unit exhibit almost identical shapes and sizes. The hydroxyl group of one of the molecules forms a hydrogen bond of 2·839 (2) Å with the hydroxyl O of the other molecule, which in turn is involved in an intramolecular O—H···π hydrogen bond with the ethynyl group.

Introduction. An extensive study has been made in our Department on 2-substituted-5-phenyladamantanes as probes to determine the stereochemical course of various reactions. In this connection, the configurations of a number of 2-substituted-5-phenyladamantanes, especially those with a 2-ethynyl group, have been determined. The present paper reports the structure of the parent alcohol, 2-ethynyl-2-adamantanol.

The diffraction data were obtained on an Enraf–Nonius CAD-4A diffractometer. The data collection range was up to 65° in θ, and the θ–2θ scan technique

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* IUPAC name: 2-ethynyltricyclo[3.3.1.1^{3,7}]decan-2-ol.

† Crystallographic Studies on Adamantanes. V.

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