

Loss of the OH group leaves a migrating 21 (22) double bond blocked by the C(28) methyl at C(17) which could then be followed by loss of the isopropyl group by chemical or biological scission. Subsequent acid hydrogenation of the 13 (18) double bond from the now less hindered α face would produce the *D/E cis* junction and yield *H*. A more complete discussion of the origin and significance of triterpanes in crude petroleum is given by Whitehead (1973*a, b*).

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The Crystal and Molecular Structure of 29-Nor-17 α H-hopane, C₂₉H₅₀

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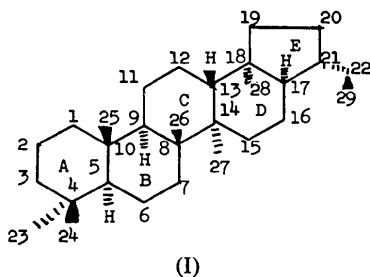
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The structure of 29-nor-17 α H-hopane (triterpane *D*) has been determined by direct methods from counter intensities. The compound is orthorhombic, space group $P2_12_12_1$, with $Z=4$, and the diffraction data were refined to $R=0.120$. The molecule is composed of four *trans*-fused six-membered chair rings, *A, B, C, D*, with a five-membered ring *E cis*-fused to ring *D*. A geminal dimethyl group is sited at C(4) with other methyl groups at C(10), C(8), C(14) and C(18) and an ethyl group at C(21).

Introduction

In two previous papers (Smith, 1970, 1975), the structures of the hitherto unknown triterpanes, *E* and *H* have been reported. A third unknown triterpane, *D*, another in a series of pentacyclic hydrocarbons extracted from a Nigerian crude petroleum (Hills & Whitehead, 1966), has been shown to be 29-nor-17 α H-hopane with formula (I).



N.m.r. evidence showed the presence of seven methyl groups and deductions had been made from mass spectrometry that compound *D* was likely to contain an ethyl group which would account for its relatively low melting point $\sim 180^\circ\text{C}$. This may be compared with the melting point of lupane $188\text{--}189^\circ\text{C}$ which possesses an isopropyl group, whereas the melting points of compounds *E* and *H*, neither of which contains rotatable groups are 260 and 233°C respectively.

Crystal data

Triterpane *D* crystallizes as orthorhombic laths or needles with the long axis parallel to *b*. Cell constants were obtained by extrapolation of successive orders of principal rows from zero-layer Weissenberg photographs taken with Cu $K\alpha$ radiation ($\lambda=1.5418 \text{ \AA}$). In addition there were sufficient high-angle reflexions on the *Ok*l layer photograph to use the method of Farquhar & Lipson (1946) for better values of *b* and *c*.

Triterpane *D*: C₂₉H₅₀, *M* = 398.40 (*C* = 12), accurate *M* by mass spectrometry 398.391; m.p. 178.0–181.0°C; *a* = 11.60 (1), *b* = 7.433 (8), *c* = 28.49 (2) Å; *U* = 2456.5 Å³; space group *P*₂₁₂₁, *Z* = 4, *D*_{*m*} = 1.07 (1), *D*_{*x*} = 1.077 g cm⁻³; $\mu(\text{Mo } K\alpha) = 0.64 \text{ cm}^{-1}$, *F*(000) = 896. Optical sign: positive. The density of the crystals was obtained by flotation in aqueous KI.

Experimental

The intensities were collected at room temperature on a PAILRED automatic diffractometer (by courtesy of Dr G. J. Bullen, University of Essex), from a crystal of approximate dimensions 0.1 × 0.1 × 0.3 mm, mounted about **b** for the layers *k* = 0 to 7. Monochromatized Mo *K*α radiation was used and within the limits of the observable diffraction pattern a total of 1662 reflexions were measured of which 173 were deemed to be unobserved. The three 0*k*0 reflexions, 020, 040 and 060 were measured by eye estimation from photographic data collected from a zero-layer Weissenberg photograph about **a** (with Mo *K*α radiation), and scaled by comparison with common reflexions. No absorption correction was made and after correction for the *L*_p factor, the unobserved reflexions were given a value corresponding to ½*F*(min) for the layer in which they occurred. An approximate scale factor and temperature factor were obtained from a Wilson plot.

Structure determination

The structure was solved by direct methods with the program *MULTAN* (Germain, Main & Woolfson, 1971). Normalized structure factors were calculated by a program developed in these laboratories from which 181 reflexions corresponding to *E* ≥ 1.5 were selected. The 200 reflexion was assigned a phase of π by similar packing considerations as occurred in the other two structures.

Two out of 16 solutions had outstandingly high figures of merit and also the lowest residuals. A comparison of the refined phase angles showed that the two solutions were in essence identical and an *E*_o map was calculated for one solution only.

From the map, 29 strong peaks were selected which satisfied the expected triterpenoid structure although these peaks did not include the expected ethyl group. In addition there were five other obviously false peaks. The 29 atom peaks corresponded to all the atoms in (1) except C(22) and C(29) plus two methyl groups in geometrically acceptable positions associated with C(13) and C(17). After three cycles of least-squares refinement both these latter methyl sites were rejected by giving the atoms very high temperature factors, and in the subsequent *F*_o and difference maps the two atoms of the ethyl group attached to C(21) were visible. A re-examination of the *E*_o map showed that these atoms were present but with much reduced peak height.

Table 1. Fractional coordinates and thermal vibration parameters for carbon atoms

The expression for the anisotropic temperature factor is $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{23}kl + \beta_{13}hl + \beta_{12}hk)]$. Standard deviations in parentheses refer to the last decimal places. Values are × 10⁴.

	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	β_{11}	β_{22}	β_{33}	β_{23}	β_{13}	β_{12}
C(1)	8115 (9)	7865 (16)	4491 (4)	103 (11)	239 (28)	18 (2)	23 (13)	-27 (8)	-94 (33)
C(2)	8079 (10)	8035 (15)	3967 (4)	112 (12)	206 (26)	17 (2)	17 (12)	-13 (8)	34 (32)
C(3)	8964 (9)	6726 (15)	3741 (3)	100 (11)	241 (28)	12 (2)	60 (12)	11 (7)	12 (31)
C(4)	8790 (10)	4797 (15)	3867 (3)	108 (11)	211 (25)	9 (1)	58 (10)	-8 (7)	89 (30)
C(5)	8766 (8)	4659 (13)	4406 (3)	55 (8)	161 (22)	13 (1)	6 (10)	-23 (6)	-10 (25)
C(6)	8674 (9)	2758 (15)	4612 (3)	96 (10)	226 (27)	12 (2)	-29 (11)	10 (7)	118 (31)
C(7)	9026 (8)	2660 (15)	5117 (3)	67 (9)	216 (25)	14 (2)	39 (13)	-9 (7)	-19 (29)
C(8)	8319 (8)	3930 (12)	5431 (3)	52 (8)	94 (18)	14 (1)	-14 (10)	9 (6)	78 (22)
C(9)	8252 (7)	5856 (12)	5202 (3)	44 (7)	90 (17)	12 (1)	-1 (9)	-18 (6)	6 (22)
C(10)	7903 (8)	5910 (13)	4675 (3)	68 (9)	114 (19)	13 (2)	14 (9)	10 (6)	62 (24)
C(11)	7501 (9)	7097 (13)	5507 (4)	76 (9)	132 (21)	18 (2)	-19 (11)	-3 (7)	110 (26)
C(12)	8002 (10)	7253 (15)	6012 (4)	126 (12)	201 (26)	15 (2)	-38 (12)	3 (8)	-14 (34)
C(13)	8175 (8)	5394 (13)	6239 (3)	61 (9)	141 (21)	13 (1)	-2 (10)	10 (6)	19 (24)
C(14)	8954 (8)	4172 (13)	5934 (3)	62 (8)	150 (20)	7 (1)	3 (9)	4 (6)	-6 (24)
C(15)	9094 (8)	2342 (13)	6178 (3)	69 (9)	154 (21)	9 (1)	4 (9)	22 (6)	99 (25)
C(16)	9499 (10)	2485 (17)	6698 (4)	94 (11)	308 (32)	15 (2)	45 (14)	5 (8)	82 (37)
C(17)	8691 (8)	3672 (13)	6982 (3)	66 (9)	176 (22)	10 (1)	-9 (10)	-17 (6)	-19 (25)
C(18)	8450 (9)	5545 (14)	6785 (3)	111 (12)	210 (26)	11 (2)	-28 (11)	-27 (7)	-79 (32)
C(19)	7389 (11)	6101 (15)	7051 (4)	144 (14)	230 (28)	13 (2)	-39 (12)	13 (9)	81 (36)
C(20)	6681 (9)	4449 (15)	7120 (4)	94 (11)	215 (27)	19 (2)	-32 (13)	19 (8)	27 (32)
C(21)	7496 (8)	2863 (15)	7074 (3)	78 (9)	250 (27)	8 (1)	19 (11)	13 (6)	1 (30)
C(22)	7517 (9)	1567 (16)	7510 (4)	74 (10)	293 (31)	13 (2)	-15 (13)	-1 (7)	-2 (32)
C(23)	9842 (11)	3764 (19)	3687 (3)	136 (14)	437 (41)	8 (2)	16 (14)	35 (8)	149 (42)
C(24)	7716 (11)	4022 (17)	3632 (4)	127 (13)	278 (30)	14 (2)	1 (13)	-10 (8)	13 (42)
C(25)	6608 (8)	5480 (14)	4587 (4)	51 (8)	209 (26)	19 (2)	3 (12)	1 (7)	-57 (27)
C(26)	7109 (7)	3053 (13)	5497 (3)	47 (8)	165 (22)	14 (2)	13 (11)	18 (6)	43 (24)
C(27)	10179 (9)	4973 (15)	5871 (3)	78 (10)	246 (26)	10 (1)	28 (11)	-13 (9)	-88 (29)
C(28)	9476 (12)	6869 (17)	6889 (4)	184 (17)	305 (35)	12 (2)	6 (14)	-13 (9)	-77 (46)
C(29)	6380 (11)	554 (18)	7578 (4)	113 (12)	362 (39)	18 (2)	-27 (16)	18 (9)	-67 (42)

Refinement

With the NRC program system (Ahmed, Hall, Pippy & Huber, 1966), the block-diagonal least-squares isotropic refinement was started for the 29 carbon atoms only, reducing R from 0.25 to 0.18. Scattering factors were taken from *International Tables for X-ray Crystallography*. At this point the positions of 29 hydrogen atoms fixed by geometry were calculated with C-H = 1.08 Å and their fixed contribution to the structure factors included. R fell to 0.164. A difference map was computed from which some of the methyl hydrogen atoms were found, and after estimating the positions of the missing ones and adjusting their geometry to trigonal symmetry around their associated carbon atoms, the inclusion of all 50 hydrogen atoms caused R to converge at 0.146. The hydrogen atoms were given the isotropic temperature factor of the carbon atom to which they were bonded. No attempt was made to refine the hydrogen coordinates. The weighting scheme used was of the type $0 \leq F_o \leq 12$, $\sqrt{w} = F_o/12$, $12 < F_o$, $\sqrt{w} = 12/F_o$.

Anisotropic refinement of carbon atoms only was started with a 9×9 matrix and the weighting scheme changed to $w^{-1} = 1 + (F_o - b)^2/a^2$ where $a = 15$ and $b = 30$. Hydrogen-atom positions were recalculated after every three cycles and inter-layer scaling carried out at intervals (Eichhorn, 1956). Before the last three cycles the methyl hydrogen atom positions were reassessed from a difference map calculated on structure factors phased without hydrogen-atom contributions. The final R for 1492 observed reflexions was 0.120 (0.134 including the unobserved reflexions) when all parameter shifts were less than six standard deviations. Positional and thermal parameters of the carbon atoms are given in Table 1 and the calculated hydrogen positions in Table 2. The observed and calculated structure factors are in Table 3.*

* Table 3 has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 30694 (12 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2. Calculated fractional coordinates and thermal parameters for the hydrogen atoms ($\times 10^4$)

The second and third digits of the hydrogen number refer to the bonded carbon atom. The positions of hydrogen atoms H(101) to H(222) are calculated positions based on a fixed geometry. Some of the positions of the methyl hydrogen atoms were taken from an F_o map and, with the remainder, their positions were adjusted to give trigonal geometry around the methyl carbon atom. The isotropic temperature factor B is the temperature factor of the bonded carbon atom at the end of the last isotropic refinement cycle.

	x/a	y/b	z/c	B
H(101)	8937	8352	4617	4.802
H(201)	7493	8768	4643	4.802
H(102)	8279	9409	3869	4.139
H(202)	7228	7708	3843	4.139

Table 2 (cont.)

H(103)	9835	7137	3845	4.215
H(203)	8953	6890	3363	4.215
H(105)	9613	5128	4515	3.061
H(106)	9176	1830	4411	3.938
H(206)	7778	2302	4583	3.938
H(107)	9925	3012	5145	3.444
H(207)	8942	1306	5244	3.444
H(109)	9117	6394	5215	2.134
H(111)	7452	8429	5348	5.062
H(211)	6626	6570	5525	5.062
H(112)	8815	7962	5996	4.489
H(212)	7432	8060	6225	4.489
H(113)	7338	4756	6226	3.534
H(115)	9706	1517	5985	2.713
H(215)	8284	1616	6166	2.713
H(116)	10361	3069	6712	5.410
H(216)	9550	1184	6860	5.410
H(117)	9098	3855	7323	3.225
H(119)	7625	6652	7390	5.470
H(219)	6907	7067	6843	5.470
H(120)	6304	4468	7463	4.848
H(220)	6039	4379	6848	4.848
H(121)	7239	2087	6772	3.634
H(122)	8212	624	7471	4.296
H(222)	7711	2351	7823	4.296
H(123)	10045	4197	3336	5.079
H(223)	9621	2315	3671	5.079
H(323)	10553	3942	3915	5.079
H(124)	7970	3177	3350	6.377
H(224)	7203	5143	3499	6.377
H(324)	7220	3291	3887	6.377
H(125)	6449	5371	4217	4.454
H(225)	6088	6570	4730	4.454
H(325)	6376	4241	4760	4.454
H(126)	6904	2254	5187	2.801
H(226)	6463	4088	5537	2.801
H(326)	7113	2193	5800	2.801
H(127)	10495	4652	5528	3.651
H(227)	10139	6415	5915	3.651
H(327)	10748	4411	6135	3.651
H(128)	10234	6437	6708	6.414
H(228)	9238	8216	6767	6.414
H(328)	9640	6931	7261	6.414
H(129)	5897	566	7256	5.913
H(229)	6557	-822	7680	5.913
H(329)	5877	1197	7852	5.913

Discussion of the structure

Before discussing the molecular structure, a comment may be made upon the unit-cell geometry of the three triterpanes, D , E and H , so far reported. In a paper upon the crystallography of some 80 steroids (Bernal, Crowfoot & Fankuchen, 1940), compounds which are related to the triterpenoids, a classification of structure types was introduced which described in simple terms the relationship between unit-cell geometry and molecular dimensions. The most common class was called a , into which these three triterpanes also fall. The b axis is a measure of the molecular width, $a \sin \beta$ a measure, often a multiple, of the molecular thickness, while c is related to the length or is a multiple of the length of the molecule. The values of b for compounds H and D are 7.462 and 7.433 Å respectively and are consistent with both molecules having closely similar structures. On the other hand, the increased $b = 7.766$ Å

for compound *E* takes into account the siting of a geminal dimethyl group at C(20) absent in the other two. The $a \sin \beta$ values of compounds *D*, *E* and *H* are 11.60, 10.98 and 10.85 Å and in each case correspond to two molecular thicknesses. The latter two values are nearly equal, as might be expected since the width of the spiro modification of the *A* ring in compound *E* is closely similar in dimensions to the *cis*-fused *E* ring in compound *H*; but the presence of the ethyl group in *D* has caused a to increase. The c axis dimension is longest in *E* where the absence of the *cis* junction plus the position of the C(24) methyl group has produced an effective molecular length of $c/2=15.02$ Å. A shorter c axis is present in *D* as a result of the *cis* junction whilst the shortest molecular length occurs in *H* as a result of the absence of an ethyl or other terminal group and the fact that the molecule lies more nearly parallel to c^* rather than c . The structure types are therefore *D*, *a*212, *H*, *a*211 and *E*, *a*212.

The ring structure of *D* is the same as that for *H*, possessing four *trans*-fused six-membered chair rings *A*, *B*, *C*, *D* with a five-membered ring *E* *cis*-fused at C(17)–C(18). A geminal dimethyl group is at C(4) and other groups are sited at C(10), C(8), C(14) and C(18), with the expected ethyl group in the α configuration at C(21). Table 4 gives the mean planes through the five rings which show that the ring structure is flexed in not quite the same way as in *H*. The angle between the mean planes of rings *A* and *B* is 15.0° compared with 14.9° in *H* but ring *C* now makes an angle of 169.7° with ring *B* and an angle of 173.7° with ring *D*. This latter ring is bent back to lie more nearly parallel to ring *B*, whereas in *H*, rings *C* and *D* are more nearly parallel. The mean plane of ring *E* is at an angle of 69.5° to that of ring *D*. Fig. 1 shows a stereoscopic view of the molecule and Fig. 2 the molecular packing looking down **b**.

The bond angles and distances are listed in Tables 5 and 6. The mean bond angle over 57 values is $110.7(3.4)^\circ$. At the 2σ level the angles C(17)–C(18)–C(19)

and C(14)–C(13)–C(18) are significantly different from the mean which with the angle C(18)–C(17)–C(21) are influenced by the strain caused by the five-membered *E* ring. Another angle, C(4)–C(5)–C(10) whose value is close to the 2σ limit, is associated with the repulsion

Table 4. Equations to the mean planes through the five rings

Ring <i>A</i>	$-0.90432X - 0.27243Y - 0.32862Z + 14.054 = 0$
Ring <i>B</i>	$-0.93428X - 0.34727Y - 0.08073Z + 11.442 = 0$
Ring <i>C</i>	$0.90717X + 0.41208Y - 0.08506Z - 8.961 = 0$
Ring <i>D</i>	$-0.90121X - 0.43278Y - 0.02288Z + 10.879 = 0$
Ring <i>E</i>	$-0.28809X - 0.15927Y - 0.94427Z + 21.961 = 0$

Table 5. Bond angles ($^\circ$)

Standard deviations are in parentheses.

C(2)–C(1)–C(10)	114.0 (9)	C(9)–C(11)–C(12)	110.8 (8)
C(1)–C(2)–C(3)	110.0 (9)	C(11)–C(12)–C(13)	111.8 (9)
C(2)–C(3)–C(4)	114.3 (9)	C(12)–C(13)–C(14)	111.5 (8)
C(3)–C(4)–C(5)	107.8 (8)	C(12)–C(13)–C(18)	111.9 (8)
C(3)–C(4)–C(23)	107.1 (9)	C(14)–C(13)–C(18)	118.2 (8)
C(3)–C(4)–C(24)	111.7 (9)	C(8)–C(14)–C(13)	107.2 (7)
C(5)–C(4)–C(23)	108.3 (8)	C(8)–C(14)–C(15)	110.5 (7)
C(5)–C(4)–C(24)	113.4 (9)	C(8)–C(14)–C(27)	110.9 (7)
C(23)–C(4)–C(24)	108.4 (9)	C(13)–C(14)–C(15)	109.1 (7)
C(4)–C(5)–C(6)	116.4 (8)	C(13)–C(14)–C(27)	112.0 (8)
C(4)–C(5)–C(10)	117.4 (8)	C(15)–C(14)–C(27)	107.2 (7)
C(6)–C(5)–C(10)	108.4 (8)	C(14)–C(15)–C(16)	113.7 (8)
C(5)–C(6)–C(7)	113.1 (8)	C(15)–C(16)–C(17)	111.1 (9)
C(6)–C(7)–C(8)	112.6 (8)	C(16)–C(17)–C(18)	116.6 (8)
C(7)–C(8)–C(9)	110.0 (7)	C(16)–C(17)–C(21)	114.9 (8)
C(7)–C(8)–C(14)	109.9 (7)	C(18)–C(17)–C(21)	104.8 (8)
C(7)–C(8)–C(26)	107.1 (7)	C(13)–C(18)–C(17)	109.3 (8)
C(9)–C(8)–C(14)	106.8 (7)	C(13)–C(18)–C(19)	110.4 (8)
C(9)–C(8)–C(26)	112.7 (7)	C(13)–C(18)–C(28)	112.3 (8)
C(14)–C(8)–C(26)	110.4 (7)	C(17)–C(18)–C(19)	102.4 (8)
C(8)–C(9)–C(10)	115.9 (7)	C(17)–C(18)–C(28)	111.3 (8)
C(8)–C(9)–C(11)	109.8 (7)	C(19)–C(18)–C(28)	110.7 (9)
C(10)–C(9)–C(11)	112.5 (7)	C(18)–C(19)–C(20)	107.0 (9)
C(1)–C(10)–C(5)	106.7 (8)	C(19)–C(20)–C(21)	106.6 (8)
C(1)–C(10)–C(9)	107.9 (8)	C(17)–C(21)–C(20)	105.9 (8)
C(1)–C(10)–C(25)	106.8 (8)	C(17)–C(21)–C(22)	111.2 (8)
C(5)–C(10)–C(9)	106.9 (7)	C(20)–C(21)–C(22)	114.6 (8)
C(5)–C(10)–C(25)	114.6 (8)	C(21)–C(22)–C(29)	112.8 (9)
C(9)–C(10)–C(25)	113.7 (7)		



Fig. 1. Stereoscopic view of triterpane *D* drawn by ORTEP (Johnson, 1965). Vibration ellipsoids scaled to 50% probability.

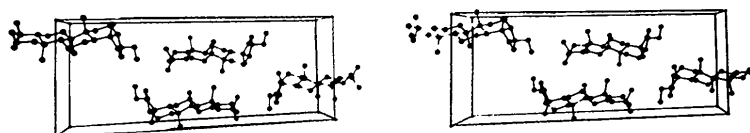


Fig. 2. Stereoscopic view showing the packing looking down **b**.

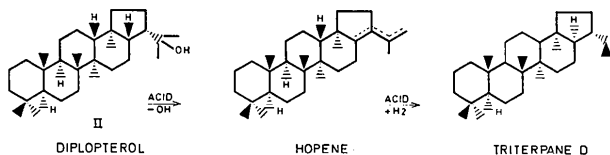
of C(25) as has been described for *H*. The mean bond distance over 33 values is 1.542 (28) Å. As with *H*, all distances except one lie within 2σ . The exception is C(8)–C(14), 1.622 Å, which is just on the 3σ limit, close to the 1.624 Å occurring in *H*, and arising no doubt from the steric strain induced by ring *E*.

Table 6. *Interatomic distances* (Å)

Standard deviations in parentheses refer to the last two decimal places.

C(1)—C(2)	1.499 (15)	C(11)—C(12)	1.557 (15)
C(1)—C(10)	1.563 (15)	C(12)—C(13)	1.538 (15)
C(2)—C(3)	1.554 (16)	C(13)—C(14)	1.549 (13)
C(3)—C(4)	1.492 (15)	C(13)—C(18)	1.590 (14)
C(4)—C(5)	1.540 (13)	C(14)—C(15)	1.537 (13)
C(4)—C(23)	1.530 (17)	C(14)—C(27)	1.551 (14)
C(4)—C(24)	1.526 (17)	C(15)—C(16)	1.558 (14)
C(5)—C(6)	1.534 (15)	C(16)—C(17)	1.519 (15)
C(5)—C(10)	1.566 (13)	C(17)—C(18)	1.527 (14)
C(6)—C(7)	1.499 (14)	C(17)—C(21)	1.534 (14)
C(7)—C(8)	1.537 (14)	C(18)—C(19)	1.504 (16)
C(8)—C(9)	1.576 (12)	C(18)—C(28)	1.572 (17)
C(8)—C(14)	1.622 (12)	C(19)—C(20)	1.490 (16)
C(8)—C(26)	1.559 (13)	C(20)—C(21)	1.517 (15)
C(9)—C(10)	1.555 (13)	C(21)—C(22)	1.572 (14)
C(9)—C(11)	1.539 (14)	C(22)—C(29)	1.531 (17)
C(10)—C(25)	1.557 (13)		

Triterpane *D* has been named 29-nor-17 α H-hopane with the implication that like *H* it originates from the older more primitive living organisms. A fuller description of the significance and origin of this compound is available (Whitehead, 1973*a, b*) but briefly a precursor for the formation of *D* could be diplopterol (22-hydroxyhopane) (II) which is known to have existed in primitive bacteria and protozoa and a possible route to its formation could be:



Under the acid-reducing conditions which exist during crude-oil maturation, the OH group would be removed leaving a migrating double bond which would come to rest at C(17)–C(21) to form hopene. Subsequent hydrogenation on the now less hindered α face would produce the *cis* *D/E* ring junction and a methyl group could eventually be lost from the isopropyl group to leave the ethyl group at C(21).

All the calculations in this study were made on a Univac 1106 computer. Permission to publish this paper has been given by The British Petroleum Company Limited and thanks are due to Messrs Hills and Whitehead of these laboratories who provided the crystals.

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