Table 2. *Bond distances* (Å), *bond angles* (°), *and selected torsion angles* (°) *with e.s.d.'s in parentheses*

N(1)–N(2)	1·275 (7)	C(8)–C(8*A*)	1·382 (9)
N(2)–N(3)	1·343 (7)	C(4*A*)–C(8*A*)	1·377 (8)
N(3)–C(4)	1·469 (8)	N(1)–C(8*A*)	1·398 (8)
C(4)–C(4*A*)	1·494 (8)	N(3)–C(31)	1·432 (9)
C(4*A*)–C(5)	1·382 (8)	C(4)–C(41)	1·516 (8)
C(5)–C(6)	1·363 (10)	C(41)–C(42)	1·505 (10)
C(6)–C(7)	1·385 (10)	C(4)–O(4)	1·418 (7)
C(7)–C(8)	1·346 (10)		
N(2)–N(1)–C(8*A*)	119·6 (5)	N(1)–C(8*A*)–C(8)	116·3 (6)
N(3)–N(2)–N(1)	121·8 (5)	N(1)–C(8*A*)–C(4*A*)	122·4 (6)
C(4)–N(3)–N(2)	126·6 (5)	C(4*A*)–C(8*A*)–C(8)	121·3 (7)
C(4*A*)–C(4)–N(3)	108·5 (5)	C(31)–N(3)–N(2)	114·4 (6)
C(5)–C(4*A*)–C(4)	121·6 (6)	C(31)–N(3)–C(4)	118·8 (6)
C(8*A*)–C(4*A*)–C(4)	120·7 (6)	O(4)–C(4)–N(3)	108·4 (5)
C(8*A*)–C(4*A*)–C(5)	117·7 (6)	O(4)–C(4)–C(4*A*)	111·2 (5)
C(6)–C(5)–C(4*A*)	121·7 (7)	C(41)–C(4)–N(3)	111·8 (5)
C(7)–C(6)–C(5)	118·7 (7)	C(41)–C(4)–C(4*A*)	111·7 (5)
C(8)–C(7)–C(6)	121·2 (7)	C(41)–C(4)–O(4)	105·2 (5)
C(8*A*)–C(8)–C(7)	119·3 (7)	C(42)–C(41)–C(4)	113·3 (7)
C(8*A*)–N(1)–N(2)–N(3)	−2·7 (1)	N(3)–C(4)–C(41)–C(42)	63·3 (1)
N(1)–N(2)–N(3)–C(4)	−0·8 (1)	C(31)–N(3)–C(4)–O(4)	−48·1 (1)
N(1)–N(2)–N(3)–C(31)	174·3 (1)	C(31)–N(3)–C(4)–C(41)	67·4 (1)
N(2)–N(3)–C(4)–C(4*A*)	6·0 (1)	N(3)–C(4)–C(4*A*)–C(8*A*)	−8·1 (1)
N(2)–N(3)–C(4)–O(4)	126·8 (1)	C(4)–C(4*A*)–C(8*A*)–N(1)	5·9 (1)
N(2)–N(3)–C(4)–C(41)	−117·7 (1)	C(4*A*)–C(8*A*)–N(1)–N(2)	0·1 (1)

the strongly puckered ring of (II) these torsion angles are −21·7, 35·0 and −26·4° respectively, while in the relatively flat (III) they are only −1·5, −2·1 and 3·7°. The title compound resembles (III) more closely than (II) with values of −0·8 (1), 6·0 (1) and −8·1 (1)°. The distortion of (II) is accompanied by some pyramidalization of its N(3), but this atom in (I) is not so affected, the sum of its bond angles at N(3) being 359·8 (10)°. The whole bicyclic system of (I) is virtually planar with deviations ranging from −0·075 to +0·045 Å. Geometry optimization of isolated molecules of (I) and (II) with *GAUSSIAN*80 tends to increase the degree of puckering: the relevant torsion angles become 18·8, −13·4 and 0·4° for (I) and −40·2, 50·2 and −28·9° for (II).

All three 4-hydroxybenzotriazines are linked by intermolecular O(4)–H(4)···N(1) hydrogen bonds. In (I) the OH···N distance of 2·762 (7) Å and OH···N angle of 173 (2)° are similar to those in the other structures. The charge-density calculation (Table 1) rules out N(2) as the proton acceptor in a hydrogen bond since it is nearly neutral. The other three heteroatoms are all candidates since they bear appreciable negative charges. However, the space around N(3) is congested with substituents, and the production of satisfactory OH···O hydrogen bonds may be incompatible with good packing of the heterocycles. Therefore N(1) appears to offer the best combination of negative charge and accessibility.

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Structure of 2β-Methyl-3-oxolupane-28-nitrile

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Abstract. $C_{31}H_{49}NO$, $M_r = 451·75$, monoclinic, $P2_1$, $a = 15·073$ (2), $b = 23·318$ (6), $c = 7·991$ (1) Å, $\beta = 104·77$ (1)°, $V = 2716·0$ (8) Å^3, $Z = 4$, $D_m = 1·098$ (5), $D_x = 1·104$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0·456$ mm^{-1}, $F(000) = 1000$, $T = 296$ K, $R = 0·041$ for 4290 unique observed reflections. The

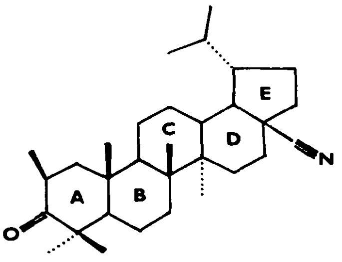
0108-2701/87/112211-04$01.50

Table 1. *Measurement and refinement data*

Crystal dimensions (mm)	0·51 × 0·40 × 0·06
No. of reflections for lattice-parameter determination	15 ($15 < \theta < 24°$)
Diffractometer	Syntex $P2_1$
Scan mode	θ–2θ
Maximum value of $(\sin\theta)/\lambda$(Å^{-1})	0·61
Standard reflections (variation)	3 after every 47 (<2%)
Absorption correction	None, $\mu = 0{\cdot}456$ mm^{-1}
$h \in$	$\langle 0,17 \rangle$
$k \in$	$\langle 0,28 \rangle$
$l \in$	$\langle -9,9 \rangle$
No. of unique reflections measured	5158
No. of reflections used $[I > 1{\cdot}96\sigma_1(I)]$	4290
Residual electron density (e Å^{-3})	0·19, −0·16
$(\Delta/\sigma)_{\max}$ for non-H atoms	0·11
for H atoms	0·23
Function minimized	$w(\lvert F_o \rvert - \lvert F_c \rvert)^2$
Weight	$\sigma^{-2}(F_o)$, derived from $\sigma(F_o)/F_o = 1/2\sigma_2(I)/I$ and $\sigma_2(I) = [\sigma_1^2(I) + (0{\cdot}06I)^2]^{1/2}$
R, wR	0·041, 0·050

asymmetric unit contains two molecules showing subtle differences in the overall geometry. In accordance with the structure in solution, the *A* ring has a distorted boat conformation.

Introduction. The title compound has been synthesized as a model for the study of *A*-ring conformations in triterpenoid ketones (Klinot, Světlý, Klinotová & Vystrčil, 1985). The NMR spectra indicated that the *A* ring adopts a boat conformation in solution (Klinot, Buděšínský, Klinotová & Vystrčil, 1986). As the geometry of the *A* ring is known to be particularly sensitive to solid-state effects, the crystal structure determination was undertaken.



Experimental. The sample was kindly provided by Professor J. Klinot. Single crystals were grown by slow evaporation of a 2% solution in benzene/hexane (1:3 v/v) at room temperature. The density was determined by flotation in an aqueous zinc bromide solution. The measurement and refinement data are summarized in Table 1. The choice of enantiomer is based on the fact that the compound belongs to a class of natural products of known chirality.

Table 2. *Final coordinates* (×10^4) *of non-*H *atoms with e.s.d.'s in parentheses*

$$B_{\rm eq} = \tfrac{4}{3}\textstyle\sum_i \sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$(Å^2)
C(101)	1564 (2)	1476 (1)	5183 (4)	3·54 (7)
C(102)	629 (2)	1612 (1)	5554 (3)	3·68 (7)
C(103)	−120 (2)	1605 (1)	3886 (3)	3·41 (7)
C(104)	−20 (2)	2046 (1)	2555 (4)	3·57 (7)
C(105)	1022 (2)	2190 (1)	2800 (3)	3·13 (6)
C(106)	1207 (2)	2504 (4)	1241 (4)	4·04 (7)
C(107)	2199 (2)	2718 (1)	1635 (4)	3·69 (7)
C(108)	2901 (2)	2221 (1)	2111 (3)	2·88 (6)
C(109)	2683 (2)	1866 (1)	3598 (3)	2·81 (6)
C(110)	1664 (2)	1666 (1)	3375 (3)	2·84 (6)
C(111)	3375 (2)	1371 (1)	4137 (4)	3·53 (7)
C(112)	4377 (2)	1577 (1)	4609 (4)	3·55 (7)
C(113)	4591 (2)	1955 (1)	3212 (3)	2·90 (6)
C(114)	3914 (2)	2474 (1)	2790 (3)	3·18 (6)
C(115)	4144 (2)	2867 (1)	1386 (5)	4·50 (8)
C(116)	5160 (2)	3031 (1)	1744 (5)	4·94 (9)
C(117)	5755 (2)	2500	2034 (4)	4·09 (8)
C(118)	5600 (2)	2155 (1)	3589 (4)	3·32 (6)
C(119)	6382 (2)	1711 (1)	3992 (4)	4·18 (8)
C(120)	6746 (2)	1561 (2)	5941 (4)	5·10 (9)
C(121)	7136 (2)	1973 (2)	3227 (6)	5·72 (11)
C(122)	6799 (2)	2570 (2)	2547 (5)	5·47 (10)
C(123)	−502 (3)	2594 (2)	3000 (6)	5·38 (11)
C(124)	−538 (2)	1861 (2)	737 (4)	4·93 (9)
C(125)	1392 (2)	1155 (1)	2148 (4)	3·58 (7)
C(126)	2829 (2)	1862 (2)	454 (4)	3·76 (7)
C(127)	4009 (2)	2850 (2)	4423 (5)	4·49 (8)
C(128)	5509 (2)	2138 (2)	451 (4)	5·27 (10)
C(129)	7170 (4)	2063 (3)	7076 (7)	8·00 (15)
C(130)	7416 (3)	1057 (3)	6130 (8)	7·73 (15)
C(131)	428 (3)	1220 (2)	6942 (4)	4·98 (9)
N(1)	5332 (3)	1867 (2)	−765 (4)	8·58 (14)
O(1)	−767 (1)	1278 (1)	3646 (3)	4·42 (5)
C(201)	−2045 (2)	4812 (1)	320 (4)	3·48 (7)
C(202)	−3032 (2)	5037 (1)	82 (4)	3·85 (7)
C(203)	−3711 (2)	4562 (1)	−565 (4)	3·83 (7)
C(204)	−3701 (2)	4331 (1)	−2353 (4)	4·20 (7)
C(205)	−2710 (2)	4377 (1)	−2607 (3)	3·46 (6)
C(206)	−2549 (2)	3985 (2)	−4031 (4)	4·21 (8)
C(207)	−1650 (2)	4115 (2)	−4475 (4)	4·11 (8)
C(208)	−807 (2)	4055 (1)	−2912 (3)	3·29 (6)
C(209)	−991 (2)	4406 (1)	−1359 (3)	2·99 (6)
C(210)	−1935 (2)	4319 (1)	−910 (3)	3·22 (6)
C(211)	−168 (2)	4364 (2)	220 (3)	3·77 (7)
C(212)	729 (2)	4556 (1)	−150 (3)	3·75 (7)
C(213)	915 (2)	4245 (1)	−1724 (3)	2·97 (6)
C(214)	87 (2)	4315 (1)	−3343 (3)	3·12 (6)
C(215)	292 (2)	3990 (2)	−4907 (3)	3·88 (7)
C(216)	1210 (2)	4144 (1)	−5269 (4)	4·09 (8)
C(217)	1988 (2)	4053 (1)	−3645 (3)	3·53 (7)
C(218)	1818 (2)	4418 (1)	−2128 (3)	3·28 (6)
C(219)	2735 (2)	4382 (1)	−702 (4)	3·74 (7)
C(220)	2995 (2)	4922 (2)	415 (4)	4·95 (9)
C(221)	3462 (2)	4210 (2)	−1694 (4)	5·02 (9)
C(222)	2963 (2)	4233 (2)	−3637 (4)	4·60 (9)
C(223)	−4350 (2)	4725 (2)	−3684 (5)	5·68 (10)
C(224)	−4102 (3)	3727 (2)	−2572 (6)	5·53 (10)
C(225)	−2008 (2)	3750 (1)	47 (4)	4·15 (8)
C(226)	−673 (3)	3409 (1)	−2465 (5)	4·51 (9)
C(227)	−45 (2)	4947 (1)	−3873 (4)	3·98 (8)
C(228)	2009 (2)	3434 (1)	−3201 (4)	3·99 (8)
C(229)	3172 (4)	5445 (2)	−594 (7)	8·12 (16)
C(230)	3824 (3)	4797 (3)	1922 (5)	6·80 (13)
C(231)	−3171 (3)	5334 (2)	1699 (6)	5·65 (11)
N(2)	2010 (2)	2955 (1)	−2945 (4)	5·85 (9)
O(2)	−4218 (2)	4378 (1)	250 (3)	5·56 (7)

Structure solution and refinement: direct methods; *F* magnitudes used in full-matrix least-squares refinement; all H atoms found from $\Delta\rho$ synthesis; scale factor, positions and temperature factors (anisotropic for non-H atoms, isotropic for H atoms) of all atoms refined in eight blocks; secondary isotropic extinction, type I, Lorentz distribution (Becker & Coppens, 1974), refined $g = 0{\cdot}17\,(2) \times 10^{-4}$; programs used: *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain,

Table 3. *Bond distances involving non-*H *atoms* (Å) *and important bond angles* (°) *with e.s.d.'s in parentheses*

	Molecule			Molecule	
	1	2		1	2
C(1)–C(2)	1·545 (4)	1·543 (4)	C(11)–C(12)	1·538 (4)	1·523 (4)
C(1)–C(10)	1·555 (4)	1·548 (4)	C(12)–C(13)	1·521 (4)	1·539 (4)
C(2)–C(3)	1·512 (3)	1·507 (4)	C(13)–C(14)	1·563 (4)	1·560 (3)
C(2)–C(31)	1·525 (5)	1·526 (6)	C(13)–C(18)	1·546 (4)	1·531 (4)
C(3)–O	1·214 (3)	1·203 (4)	C(14)–C(15)	1·554 (5)	1·557 (4)
C(3)–C(4)	1·515 (4)	1·532 (4)	C(14)–C(27)	1·547 (5)	1·532 (4)
C(4)–C(5)	1·570 (4)	1·561 (4)	C(15)–C(16)	1·534 (4)	1·528 (5)
C(4)–C(23)	1·554 (5)	1·550 (5)	C(16)–C(17)	1·512 (5)	1·526 (4)
C(4)–C(24)	1·525 (4)	1·526 (5)	C(17)–C(18)	1·547 (4)	1·556 (4)
C(5)–C(6)	1·531 (4)	1·527 (4)	C(17)–C(22)	1·531 (4)	1·527 (5)
C(5)–C(10)	1·552 (4)	1·554 (3)	C(17)–C(28)	1·487 (5)	1·483 (4)
C(6)–C(7)	1·530 (4)	1·516 (5)	C(18)–C(19)	1·540 (4)	1·554 (3)
C(7)–C(8)	1·530 (4)	1·544 (3)	C(19)–C(20)	1·554 (5)	1·535 (5)
C(8)–C(9)	1·550 (4)	1·571 (4)	C(19)–C(21)	1·547 (6)	1·559 (5)
C(8)–C(14)	1·598 (3)	1·594 (4)	C(20)–C(29)	1·518 (7)	1·523 (7)
C(8)–C(26)	1·547 (4)	1·548 (4)	C(20)–C(30)	1·531 (6)	1·525 (5)
C(9)–C(10)	1·571 (3)	1·566 (4)	C(21)–C(22)	1·532 (6)	1·544 (4)
C(9)–C(11)	1·541 (4)	1·530 (3)	C(28)–N	1·133 (5)	1·138 (4)
C(10)–C(25)	1·532 (4)	1·549 (4)			
C(2)–C(1)–C(10)	115·4 (2)	115·5 (2)	C(12)–C(13)–C(14)	111·0 (2)	110·8 (2)
C(1)–C(2)–C(3)	110·0 (2)	110·0 (2)	C(14)–C(13)–C(18)	111·4 (2)	111·3 (2)
C(2)–C(3)–C(4)	115·3 (2)	114·3 (3)	C(8)–C(14)–C(13)	107·5 (2)	108·8 (2)
C(2)–C(3)–O	122·3 (3)	123·2 (3)	C(13)–C(14)–C(15)	111·0 (2)	109·6 (2)
C(4)–C(3)–O	122·4 (2)	122·6 (3)	C(14)–C(15)–C(16)	114·1 (3)	114·4 (2)
C(3)–C(4)–C(5)	109·4 (2)	109·5 (2)	C(15)–C(16)–C(17)	110·4 (3)	110·0 (3)
C(4)–C(5)–C(10)	113·5 (2)	114·3 (2)	C(16)–C(17)–C(18)	110·1 (3)	110·0 (2)
C(5)–C(6)–C(7)	111·1 (2)	112·1 (3)	C(18)–C(17)–C(22)	101·3 (2)	101·3 (2)
C(6)–C(7)–C(8)	112·1 (2)	113·1 (2)	C(17)–C(18)–C(19)	104·6 (2)	104·4 (2)
C(7)–C(8)–C(9)	108·8 (2)	108·5 (2)	C(18)–C(19)–C(21)	104·6 (3)	104·5 (2)
C(8)–C(9)–C(10)	117·6 (2)	117·9 (2)	C(19)–C(20)–C(29)	114·3 (4)	113·7 (3)
C(8)–C(9)–C(11)	110·7 (2)	110·4 (2)	C(19)–C(20)–C(30)	109·1 (4)	109·8 (3)
C(1)–C(10)–C(5)	107·4 (2)	108·1 (2)	C(29)–C(20)–C(30)	111·5 (3)	110·6 (4)
C(5)–C(10)–C(9)	108·5 (2)	108·3 (2)	C(19)–C(21)–C(22)	106·8 (3)	106·1 (3)
C(9)–C(11)–C(12)	112·8 (2)	113·2 (2)	C(17)–C(22)–C(21)	102·9 (3)	102·5 (3)
C(11)–C(12)–C(13)	112·3 (2)	112·1 (2)	C(17)–C(28)–N	178·9 (4)	176·6 (3)

Declercq & Woolfson, 1980), *TLS* system (Sklenář & Petříček, 1973) modified for Siemens 7536.*

Discussion. The compound crystallizes with two crystallographically independent but chemically almost identical molecules in the asymmetric unit. The final coordinates are listed in Table 2 and bond distances and angles are compared in Table 3. Fig. 1 depicts a perspective view of one molecule together with the atom numbering. The unit-cell contents are depicted in Fig. 2.

The bond distances and angles lie in the normal range and display a close parallel between equivalents in the two molecules. The C–C and C–H distances average 1·539 (18), 0·98 (4) and 1·541 (21), 0·97 (4) Å for molecules 1 and 2 respectively. Only two C–C bond lengths in each molecule lie outside the 3σ limit of the mean: (*a*) as usual, the electron-withdrawing effect of the nitrile group markedly shortens the adjacent C(17)–C(28) bond; (*b*) as in many triterpenoid structures, the C(8)–C(14) distance exceeds 1·59 Å [together with less remarkable lengthening of the C(8)–C(9) and C(9)–C(10) bonds], the effect being attributable to the strain imposed by the 1,3-diaxial methyl groups [for a discussion see Langs, Duax, Carrell, Berman & Caspi (1977) or Fowell, Melsom & Smith (1978)]. The overall conformations of the rings are also identical for both molecules and correspond to distorted boat, chair, chair, chair and distorted envelope for the *A, B, C, D* and *E* rings respectively; all ring junction are *trans*.

Molecules 1 and 2 differ appreciably with respect to torsion angles. As demonstrated by Fig. 3, this effect is especially marked for the *A* and *E* rings, as is common for many similar flexible molecules crystallizing with two different conformers in the asymmetric unit [for a review, see Duax, Weeks & Rohrer (1976) and for a discussion of possible reasons and consequences see Duax, Strong & Rohrer (1980)]. The differences in the torsion angles are cumulative so that molecules 1 and 2

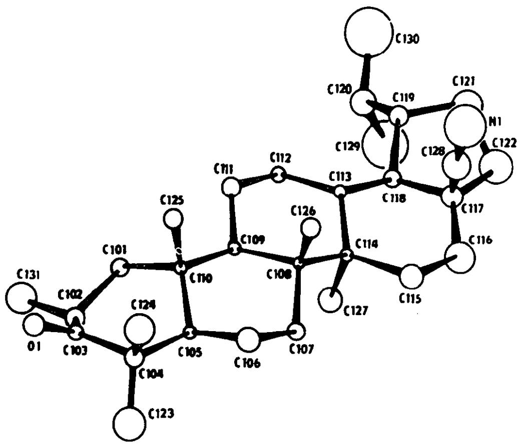


Fig. 1. Perspective view of molecule 1 with atom numbering. H atoms (omitted for clarity) are given the numbers of their bonding partners.

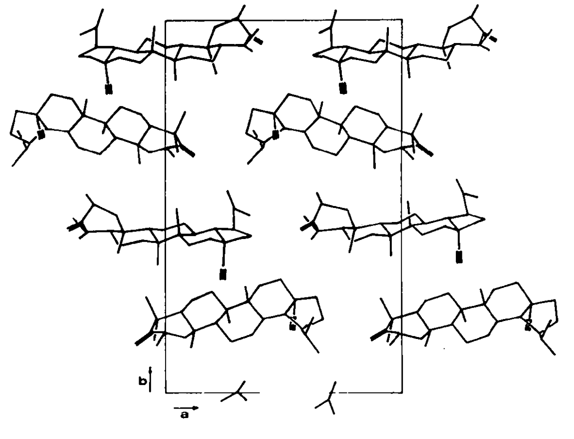


Fig. 2. Unit-cell contents projected onto the *ab* plane. The molecules are arranged in the order 1,2,1,2 along the *b* axis.

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* Lists of structure factors, anisotropic temperature factors, least-squares planes, H-atom coordinates and selected torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44154 (33 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

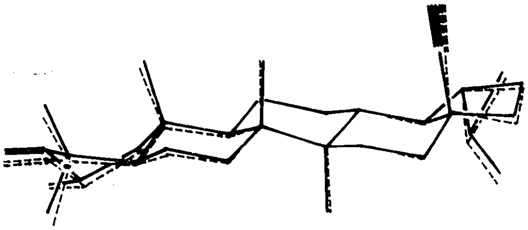

Fig. 3. Relative conformations of molecules 1 and 2 (dashed lines) illustrated by superimposing the *C* ring as a reference element.

differ further by a twist about the length of the triterpenoid skeleton. This effect is probably best measured by the pseudo torsion angle C(25)—C(10)—C(14)—C(27) which has values of −170·2 (4) and −174·3 (4)° for molecules 1 and 2 respectively.

The structure is characterized by a relatively dense packing with numerous intermolecular contacts in the usual van der Waals range. On close inspection it appears that dissimilarities in the surroundings of molecules 1 and 2 can be clearly related to the differences in their intramolecular geometry. Crystal-packing effects can therefore easily be the factor responsible for the slightly different conformations of the two independent molecules in the present structure.

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Structure of 2α-Methyl-3-oxolupane-28-nitrile

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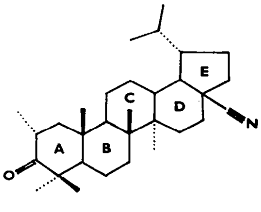
Abstract. $C_{31}H_{49}NO$, $M_r = 451\cdot75$, orthorhombic, $P2_12_12_1$, $a = 14\cdot414\ (4)$, $b = 17\cdot631\ (7)$, $c = 10\cdot631\ (2)$ Å, $V = 2702\ (1)$ Å^3, $Z = 4$, $D_m = 1\cdot094\ (8)$, $D_x = 1\cdot110\ (1)$ Mg m^{-3}, $\lambda(\text{Mo}\ K\alpha) = 0\cdot71069$ Å $\mu = 0\cdot061$ mm^{-1}, $F(000) = 1000$, $T = 296$ K, $R = 0\cdot0757$ for 1759 unique observed reflections. The most important feature of the structure is the nearly ideal chair conformation of the triterpenoid *A* ring. The *B, C, D* and *E* rings are in the usual chair, chair, chair and distorted envelope conformations, respectively, with ring junctions all *trans*. The triterpenoid skeleton is bent into a shallow V shape.

Introduction. The study of the title compound was carried out as a continuation of a comparative study of *A*-ring conformation in triterpenoid ketones both in solution (Klinot, Buděšínský, Klinotová & Vystrčil, 1986) and in the solid state (Podlahová, Podlaha, Malý & Petříček, 1987).



Experimental. The sample was kindly provided by Professor J. Klinot. Single crystals were grown by slow evaporation of a 1% solution in benzene/octane (1:5 v/v) at room temperature. Under these conditions, two modifications co-crystallize as tiny needles and well formed bipyramids which can be easily separated by

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