Watson–Crick base pairs have been found with propeller twist angles of up to 25° in double-helical DNA (Drew & Dickerson, 1981), and in $tRNA^{phe}$ (Westhof & Sundaralingam, 1986). The purine–purine G(26)–A(44) base pair in tNRA has been found to exhibit a larger twist angle of about 35°. The present structure, which is an example of a purine–purine self pair, shows a twist angle considerably greater than any previously observed. The weaker hydrogen-bonding interactions inherent to the non-Watson–Crick base pairs probably permit the higher propeller twist angles. Large twist angles may also be encountered for Watson–Crick base pairs when normal stacking interactions are disrupted, for example during transitions between right- and left-handed helices.

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Crystal Studies of Musk Compounds. III. Structures of 6-Acetyl-1,1,2,3,3,5-hexamethylindan (Musk Phantolid) (I) and 6-Acetyl-3-isopropyl-1,1,3,5-tetramethylindan (II)

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Abstract. (I), $C_{17}H_{24}O$, $M_r = 244·38$, monoclinic, $P2_1/c$, $a = 10·3130\ (7)$, $b = 14·292\ (2)$, $c = 10·6086\ (8)$ Å, $\beta = 99·135\ (7)°$, $V = 1543·8\ (3)$ Å^3, $Z = 4$, $D_x = 1·05$ Mg m^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1·5418$ Å, $\mu = 0·451$ mm^{-1}, $F(000) = 536$, room temperature, final $R = 0·056$ for 1684 observed reflections. (II), $C_{18}H_{26}O$, $M_r = 258·40$, orthorhombic, $Pbca$, $a = 10·313\ (1)$, $b = 11·049\ (2)$, $c = 28·024\ (5)$ Å, $V = 3193·3\ (9)$ Å^3, $Z = 8$, $D_x = 1·07$ Mg m^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1·5418$ Å, $\mu = 0·457$ mm^{-1}, $F(000) = 1136$, room temperature, final $R = 0·044$ for 2211 observed reflections. The aromatic ring is essentially planar in both compounds, whereas the conformation of the five-membered ring is an almost ideal C(2) envelope in (I) but is a distorted C(2) envelope in (II). The orientation of the acetyl group relative to the aromatic ring is different in (I) and (II). The geometry of the common non-H atoms is compared.

Introduction. This paper is the third in a series dealing with musk compounds [(I) and (II): De Ridder, Goubitz & Schenk (1990*a*,*b*)]. Most known synthetic aromatic musks may be classified by structure into two families according to whether they contain nitro groups (nitromusks) or not. Benzenes, indans and tetralins occur in both families but the non-nitromusks also include hydrindacene and hydrindacenone, naphthindan and naphthindanone, isochroman, coumarin and polycyclic derivatives. During the last few years, the search for new musk

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compounds has shifted towards the non-nitromusks since, from about 1980 onwards, the use of nitromusks has been put into question because it was suspected that they might have phototoxic and photoallergic properties and might possibly even cause liver cancer. The first compound described in this paper, musk phantolid, was discovered in the early 1950's by Kurt Fuchs (Wood, 1968). Like musk tonalid, its success can be attributed to its excellent odour and fixative properties in which it simulates the macrocyclic musks in their outstanding stability toward alkali and light. The second compound is a higher homolog of the indan group and has no musk odour.

Experimental. The intensities were collected with an Enraf–Nonius CAD-4 diffractometer using graphite-monochromated Cu $K\alpha$ radiation and ω–2θ scans. Preliminary Weissenberg photographs indicated the crystals of compound (I) to be monoclinic and those of compound (II) to be orthorhombic.

Structure (I): A crystal with dimensions 0·10 × 0·10 × 0·05 mm was used for data collection. 2599 unique reflections within the ranges $2{\cdot}5 \le \theta \le 75°$, $0 \le h \le 8$, $0 \le k \le 17$, $-13 \le l \le 13$ were measured, of which 1684 were above the significance level of $2{\cdot}5\sigma(I)$. Two standard reflections, 022 and $21\bar{1}$, measured hourly, suffered a 25·4% decrease during 36 h collection time and this was corrected for. Unit-cell parameters were refined by a least-squares algorithm using 23 reflections with $79 < 2\theta < 90°$. Absent reflections $h0l$, $l \ne 2n+1$ and $0k0$, $k \ne 2n+1$ indicated the space group $P2_1/c$. Corrections applied for Lorentz and polarization effects, not for absorption. Structure determined by direct methods using the program *SIMPEL*83 (Schenk & Kiers, 1983). The H-atom positions were initially calculated on the basis of standard geometry. The coordinates of all H atoms except H(2) were refined. Block-diagonal least-squares refinement on F, anisotropic for the non-H atoms and isotropic for the H atoms, converged to $R = 0{\cdot}057$, $wR = 0{\cdot}071$, $S = 0{\cdot}16$. Max. $\Delta/\sigma = 0{\cdot}95$. A weighting scheme $w^{-1} = 8{\cdot}76 + F_{\rm obs} + 0{\cdot}0057F_{\rm obs}^2$ was used. The isotropic secondary-extinction coefficient refined to $1{\cdot}10\,(9) \times 10^{-6}$ (Larson, 1967). A final difference synthesis revealed a residual electron density between 0·0 and 0·4 e Å^{-3}.

Structure (II): Crystal dimensions 0·50 × 0·33 × 0·23 mm. 3032 unique reflections were measured within the ranges $2{\cdot}5 \le \theta \le 70°$, $0 \le h \le 12$, $0 \le k \le 12$, $0 \le l \le 34$. Of these 2211 were above the significance level of $2{\cdot}5\sigma(I)$. The intensities of two standard reflections, 232 and 046, measured hourly, showed no significant decrease during 39 h collection time. Unit-cell parameters were refined by a least-squares fitting procedure using 23 reflections with $84 < 2\theta < 90°$. Absent reflections $0kl$, $k \ne 2n+1$, $h0l$, $l \ne 2n+1$ and $hk0$, $h \ne 2n+1$ indicated the space group $Pbca$. Corrections were applied for Lorentz and polarization effects, not for absorption. The structure was determined by direct methods using the program *SIMPEL*83 (Schenk & Kiers, 1983). The H-atom positions were calculated on the basis of standard geometry. Block-diagonal least-squares refinement on F, anisotropic for the non-H atoms and isotropic for the H atoms, converged to $R = 0{\cdot}044$, $wR = 0{\cdot}058$, $S = 0{\cdot}17$. Max. Δ/σ was 0·74. A weighting scheme $w^{-1} = 10{\cdot}7 + F_{\rm obs} + 0{\cdot}0044F_{\rm obs}^2$ was used. The isotropic secondary-extinction coefficient refined to $2{\cdot}4\,(1) \times 10^{-6}$ (Larson, 1967). A final difference synthesis revealed a residual electron density between −0·1 and 0·2 e Å^{-3}.

All calculations were performed with *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) unless stated otherwise. The scattering factors were taken from Cromer & Mann (1968) and *International Tables for X-ray Crystallography* (1974, Vol. IV).

Discussion. A uniform numbering system was used for both molecules: molecule (I) has two methyl groups on C(1) and one on C(2) whereas molecule (II) has a methyl and an isopropyl group on C(1) but no non-hydrogen substituents on C(2). Final positional parameters for the non-H atoms for both structures are listed in Table 1.* Bond lengths and angles are given in Table 2 and have normal values. *PLUTO* (Motherwell & Clegg, 1978) drawings of the molecules showing the atomic numbering scheme are given in Fig. 1 [for structure (I)] and Fig. 2 [for structure (II)].

The aromatic ring is essentially planar within the limits of accuracy in both molecules. Following the criteria defined by Altona, Geise & Romers (1968), the non-aromatic ring is classified as an almost ideal C(2) envelope for compound (I) and a distorted C(2) envelope for compound (II) [(I): $\varphi_m = 23{\cdot}8°$, $\Delta = 34{\cdot}8°$ and (II): $\varphi_m = 19{\cdot}4°$, $\Delta = 17{\cdot}7°$]. The torsion angle C(6)—C(5)—C(15)—O(1) is 21·1 (4)° in (I) and 4·5 (3)° in (II). The equivalent angle in musk tonalid is 22° (De Ridder *et al.*, 1990*b*). The intramolecular distances C(17)···O(1) and H(171)···O(1) are respectively 2·826 (6) and 2·37 (4) Å for (I) and 2·739 (3) and 2·43 (3) Å for (II).

In both structures there are no intermolecular distances significantly shorter than the sum of the van der Waals radii. The shortest intermolecular distance in (I) is 3·544 (4) Å [O(1)···C(16), symmetry

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53573 (36 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional coordinates of the non-*H *atoms and equivalent isotropic thermal parameters* (Å^2)

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

	x	y	z	U_{eq}
Compound (I)				
C(1)	0·6409 (3)	0·6206 (2)	0·1572 (3)	0·064 (2)
C(2)	0·6107 (4)	0·5587 (3)	0·2688 (4)	0·099 (3)
C(3)	0·7118 (3)	0·4778 (2)	0·2883 (3)	0·065 (2)
C(4)	0·8183 (3)	0·4020 (2)	0·1063 (2)	0·054 (2)
C(5)	0·8444 (3)	0·4074 (2)	−0·0192 (2)	0·053 (2)
C(6)	0·8049 (3)	0·4875 (2)	−0·0930 (2)	0·058 (2)
C(7)	0·7401 (3)	0·5586 (2)	−0·0383 (3)	0·061 (2)
C(8)	0·7130 (3)	0·5513 (2)	0·0846 (2)	0·053 (2)
C(9)	0·7519 (3)	0·4733 (2)	0·1573 (2)	0·051 (2)
C(10)	0·5108 (4)	0·6525 (3)	0·0770 (4)	0·095 (3)
C(11)	0·7241 (4)	0·7076 (2)	0·1921 (4)	0·094 (3)
C(12)	0·5820 (5)	0·6095 (3)	0·3867 (4)	0·123 (4)
C(13)	0·6452 (5)	0·3871 (3)	0·3209 (4)	0·115 (3)
C(14)	0·8344 (5)	0·4961 (4)	0·3883 (3)	0·117 (3)
C(15)	0·9098 (3)	0·3254 (2)	−0·0707 (3)	0·068 (2)
C(16)	0·9876 (4)	0·2598 (2)	0·0207 (4)	0·089 (2)
C(17)	0·8288 (4)	0·5003 (3)	−0·2292 (3)	0·096 (3)
O(1)	0·8999 (3)	0·3109 (2)	−0·1839 (2)	0·112 (2)
Compound (II)				
C(1)	0·4071 (2)	0·2558 (2)	0·07320 (7)	0·042 (1)
C(2)	0·5392 (2)	0·1891 (2)	0·07600 (7)	0·047 (1)
C(3)	0·5471 (2)	0·1212 (2)	0·12405 (7)	0·041 (1)
C(4)	0·3501 (2)	0·0461 (2)	0·17460 (6)	0·0364 (9)
C(5)	0·2173 (2)	0·0553 (2)	0·18464 (6)	0·0361 (9)
C(6)	0·1407 (2)	0·1382 (2)	0·15855 (6)	0·0391 (9)
C(7)	0·1989 (2)	0·2043 (2)	0·12205 (6)	0·0408 (9)
C(8)	0·3292 (2)	0·1913 (2)	0·11141 (6)	0·0360 (9)
C(9)	0·4055 (2)	0·1141 (2)	0·13842 (6)	0·0353 (9)
C(10)	0·4203 (2)	0·3900 (2)	0·08757 (8)	0·059 (1)
C(11)	0·3413 (2)	0·2458 (2)	0·02359 (7)	0·048 (1)
C(13)	0·6095 (2)	−0·0035 (2)	0·11883 (8)	0·056 (1)
C(14)	0·6225 (2)	0·1938 (2)	0·16212 (8)	0·059 (1)
C(15)	0·1611 (2)	−0·0257 (2)	0·22185 (6)	0·044 (1)
C(16)	0·2425 (2)	−0·1204 (2)	0·24445 (9)	0·067 (1)
C(17)	−0·0023 (2)	0·1578 (2)	0·16765 (8)	0·058 (1)
C(111)	0·3041 (2)	0·1165 (2)	0·01025 (8)	0·060 (1)
C(112)	0·4212 (3)	0·3027 (2)	−0·01623 (8)	0·072 (2)
O(1)	0·0486 (2)	−0·0192 (2)	0·23347 (7)	0·100 (1)

operation $x, \frac{1}{2}-y, -\frac{1}{2}+z$] and 3·369 (3) Å in (II) [O(1)···C(4), through symmetry operation $\frac{1}{2}+x, y, \frac{1}{2}-z$]. The relatively shorter intermolecular distances in the latter may explain the distortion in the five-membered ring.

Matching of the common non-H atoms resulted in an r.m.s. value of 0·21 Å. This is mainly caused by the significantly different twisting-out angles of the acetyl group *versus* the aromatic ring [the largest difference is observed at the atoms C(16) and O(1) with a distance of 0·62 and 0·49 Å, respectively]. Structure (II) is structurally isomeric with musk tonalid, the structure of which has been reported previously (De Ridder *et al.*, 1990*b*). The observation that compound (II) has no musk odour indicates the important influence of the molecular shape in the structure–activity relationship.

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

	(I)	(II)
C(1)—C(2)	1·549 (5)	1·551 (3)
C(1)—C(8)	1·519 (4)	1·516 (2)
C(1)—C(10)	1·539 (5)	1·542 (3)
C(1)—C(11)	1·523 (5)	1·551 (3)
C(2)—C(3)	1·548 (5)	1·544 (3)
C(2)—C(12)	1·515 (6)	–
C(3)—C(9)	1·513 (4)	1·517 (2)
C(3)—C(13)	1·531 (6)	1·528 (3)
C(3)—C(14)	1·539 (5)	1·545 (3)
C(4)—C(5)	1·401 (4)	1·402 (2)
C(4)—C(9)	1·385 (4)	1·384 (2)
C(5)—C(6)	1·410 (4)	1·413 (2)
C(5)—C(15)	1·498 (4)	1·492 (2)
C(6)—C(7)	1·394 (4)	1·393 (3)
C(6)—C(17)	1·515 (4)	1·513 (3)
C(7)—C(8)	1·380 (4)	1·384 (2)
C(8)—C(9)	1·379 (4)	1·386 (2)
C(11)—C(111)	–	1·525 (3)
C(11)—C(112)	–	1·524 (3)
C(15)—C(16)	1·488 (5)	1·483 (3)
C(15)—O(1)	1·208 (4)	1·207 (2)
C(2)—C(1)—C(8)	100·9 (2)	101·9 (1)
C(2)—C(1)—C(10)	109·2 (3)	111·4 (2)
C(2)—C(1)—C(11)	117·0 (3)	113·3 (2)
C(8)—C(1)—C(10)	111·5 (3)	108·3 (2)
C(8)—C(1)—C(11)	110·7 (3)	111·6 (1)
C(10)—C(1)—C(11)	107·4 (3)	110·0 (2)
C(1)—C(2)—C(3)	108·4 (3)	108·7 (1)
C(1)—C(2)—C(12)	116·5 (3)	–
C(3)—C(2)—C(12)	117·6 (3)	–
C(2)—C(3)—C(9)	100·7 (2)	101·9 (1)
C(2)—C(3)—C(13)	110·2 (3)	112·2 (2)
C(2)—C(3)—C(14)	115·3 (3)	112·1 (2)
C(9)—C(3)—C(13)	111·7 (3)	112·6 (2)
C(9)—C(3)—C(14)	109·0 (3)	109·2 (1)
C(13)—C(3)—C(14)	109·7 (3)	108·8 (2)
C(5)—C(4)—C(9)	120·8 (2)	120·7 (2)
C(4)—C(5)—C(6)	119·4 (3)	119·3 (2)
C(4)—C(5)—C(15)	118·0 (2)	118·4 (2)
C(6)—C(5)—C(15)	122·6 (2)	122·3 (2)
C(5)—C(6)—C(7)	118·4 (2)	118·7 (2)
C(5)—C(6)—C(17)	123·5 (3)	123·4 (2)
C(7)—C(6)—C(17)	118·0 (3)	117·9 (2)
C(6)—C(7)—C(8)	121·4 (2)	121·4 (2)
C(1)—C(8)—C(7)	128·2 (2)	128·1 (2)
C(1)—C(8)—C(9)	111·4 (2)	112·0 (1)
C(7)—C(8)—C(9)	120·3 (3)	119·8 (2)
C(3)—C(9)—C(4)	127·9 (2)	128·3 (2)
C(3)—C(9)—C(8)	112·5 (2)	111·7 (1)
C(4)—C(9)—C(8)	119·6 (2)	120·0 (2)
C(1)—C(11)—C(111)	–	113·4 (2)
C(1)—C(11)—C(112)	–	113·0 (2)
C(111)—C(11)—C(112)	–	110·1 (2)
C(5)—C(15)—C(16)	118·9 (3)	120·2 (2)
C(5)—C(15)—O(1)	121·7 (3)	121·7 (2)
C(16)—C(15)—O(1)	119·4 (3)	118·1 (2)

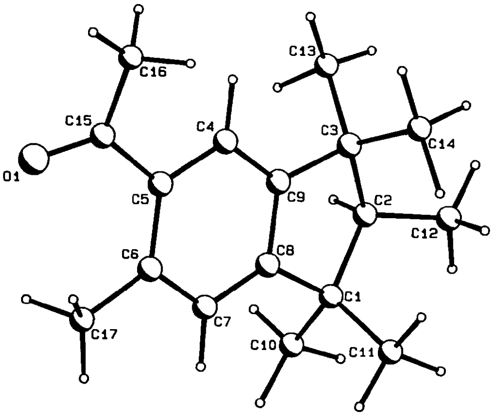

Fig. 1. The numbering system of musk phantolid (I). The H atoms are shown but not labelled.

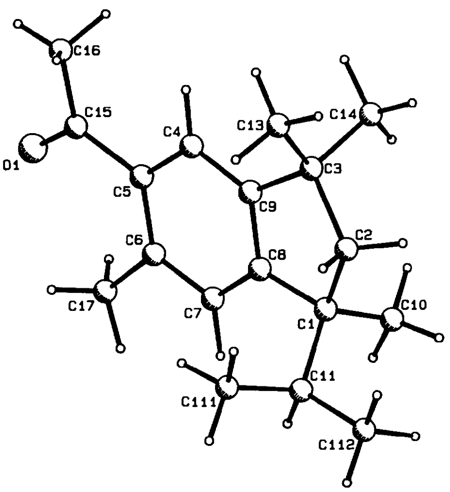

Fig. 2. The numbering system of 6-acetyl-3-isopropyl-1,1,3,5-tetramethylindan (II). The H atoms are shown but not labelled.

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trans-4-*tert*-Butyl-3-hydroxy-5-cyclohepten-1-one (2) and *trans*-6-*tert*-Butyl-3-hydroxy-2,7-dimethyl-4-cyclohepten-1-one (5)

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Abstract. (2) $C_{11}H_{18}O_2$, $M_r = 182{\cdot}3$, monoclinic, $P2_1/a$, $a = 7{\cdot}463\,(3)$, $b = 9{\cdot}776\,(3)$, $c = 14{\cdot}955\,(5)$ Å, $\beta = 97{\cdot}33°$, $V = 1082{\cdot}2$ Å^3, $Z = 4$, $D_x = 1{\cdot}12$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}70$ cm^{-1}, $F(000) = 400$, room temperature, $R = 0{\cdot}041$ for 480 observed reflections. (5) $C_{13}H_{22}O_2$, $M_r = 210{\cdot}3$, orthorhombic, $Pnab$, $a = 9{\cdot}747\,(1)$, $b = 10{\cdot}724\,(2)$, $c = 24{\cdot}365\,(4)$ Å, $V = 2546{\cdot}8$ Å^3, $Z = 8$, $D_x = 1{\cdot}10$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}67$ cm^{-1}, $F(000) = 928$, room temperature, $R = 0{\cdot}037$ for 521 observed reflections. In both (2) and (5) the hydroxyl group is *trans* with respect to the *tert*-butyl group. In (2) pairs of molecules are linked *via* hydrogen bonds [O···O $(1-x,\ 1-y,\ 1-z)$ 2·809 (7) Å] to form centrosymmetric dimers, while in (5) molecules are hydrogen bonded [O···O$(x,\ -0{\cdot}5+y,\ 1{\cdot}5-z)$ 2·847 (7) Å] through 2_1 screw axes to form infinite chains. The highly strained seven-membered ring in (2) has a boat-type conformation and in (5) it has a sofa-type conformation.

Introduction. We have recently investigated the ring opening reaction of 8-oxabicyclo[3.2.1]oct-6-en-3-one (1) and 2,4-dimethyl-8-oxabicyclo[3.2.1]oct-6-en-3-one (4) with organocuprate reagents (Lautens, Di Felice & Huboux, 1989). These types of reaction provide an extremely efficient route to seven-membered rings where two or four contiguous stereocentres are created in two steps. The syntheses of the starting oxabicyclic compounds (1) and (4) were carried out according to a literature procedure (Fohlisch, Gottstein, Herter & Wanner, 1981; Hoffmann, 1984). Treatment of compound (1) with five equivalents of ^{t}BuLi/CuCN (1·6/1) in tetrahydrofuran with ageing the cuprate for 3 h led to the formation of the regioisomers (2) and (3) in 3/1 ratio with total yield of 95%. Under the same experi-

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