S(4)—C(5x)—C(6x)—S(1ⁱ)	−175.5 (12)
C(5)—C(6x)—S(1ⁱ)—C(2xʲ)	−55.3 (21)
C(5x)—C(6)—S(1ⁱ)—C(2ⁱ)	84.1 (16)
C(5x)—C(6x)—S(1ⁱ)—C(2xʲ)	119.0 (23)
C(6ⁱ)—S(1)—C(2x)—C(3x)	78 (3)
C(6xⁱ)—S(1)—C(2)—C(3)	−63.7 (13)
C(6xⁱ)—S(1)—C(2x)—C(3x)	109 (3)

In the iodine molecule

I(7)—I(7ⁱⁱ)	2.736 (1)

Between the molecules

S(1)—I(7)	3.220 (3)

S(1)—I(7)—I(7ⁱⁱ)	170.5 (1)	C(2x)—S(1)—I(7)	128.8 (16)
C(2)—S(1)—I(7)	89.2 (4)	C(6xⁱ)—S(1)—I(7)	118.5 (8)
C(6ⁱ)—S(1)—I(7)	79.6 (6)		

Symmetry codes: (i) $1 - x, -y, 1 - z$; (ii) $-x, -y, -z$.

Table 3. *Calculated bonding parameters for* Me₂S, I₂ *and their CT complexes*

	Bond orders			Net electron	Bond lengths (Å)		
	I—I	S—I	C—S	transfer (e)	I—I	S—I	C—S
I₂	1.00	–	–	–	2.668	–	–
Me₂S	–	–	1.00	–	–	–	1.801
Me₂S.I₂	0.76	0.23	0.98	0.20	2.690	2.707	1.810
(Me₂S)₂.I₂	0.74	0.12	0.99	0.25	2.696	2.767	1.808

The ethylene bridges are disordered, each in two possible orientations. In the final cycles of refinement, the C atoms of the more populated arrangements were refined anisotropically, those of the minor sites isotropically. For the major ethylene groups, H atoms were included in calculated positions but with freely refined U_{iso}'s. The site occupancy factors of the disordered groups were refined, in one bridge to 0.85/0.15 (3) and in the other bridge to 0.65/0.35 (3).

The structure was determined by a combination of heavy-atom, direct and trial-and-error methods with the *SHELX*76 (Sheldrick, 1976) and *SHELXS*86 (Sheldrick, 1985) programs. Refinement was by full-matrix least-squares methods in *SHELX*76.

Computer programs, noted above and by Anderson, Richards & Hughes (1986) were run on a MicroVAXII computer.

We thank the SERC for a CASE award to SDH.

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Two Highly Substituted Methylenecyclopropanes

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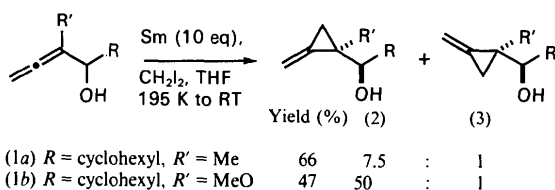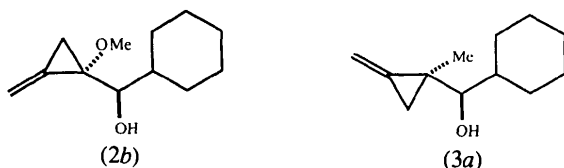
Abstract

The relative stereochemistries of the two title compounds, (R^*,R^*)-α-(1-methoxy-2-methylenecyclopropyl)-cyclohexanemethanol (2b), $C_{12}H_{20}O_2$, and (R^*,R^*)-α-(1-methyl-2-methylenecyclopropyl)cyclohexanemethanol (3a), $C_{12}H_{20}O$, have been established. Each structure has a different mode of hydrogen bonding; compound (2b) forms infinite chains [O⋯O 2.862 (3) Å], while compound (3a) forms centrosymmetric tetramers [O⋯O 2.782 (4) and 2.835 (4) Å].

Comment

Methylenecyclopropanes are among the most highly strained carbocyclic molecules (Greenberg & Liebman, 1978) and have attracted attention from the synthetic (Ohta & Takaya, 1991), mechanistic (Dewar & Wasson, 1971) and biological perspectives (Baldwin & Widdison, 1992). We have recently reported a novel highly regioselective cyclopropanation of α-allenic alcohols (1) using samarium/dihalomethane to provide a variety of methylene- and alkylidenecyclopropane carbinols [compounds (2) and (3)] in good yields (Lautens & Delanghe, 1993, 1994). The diastereoselectivity varies from 1:1 to 50:1 and depends on the substituents on the carbinol side chain (R group) and on the substitution of the allene (R' group).

(1a) R = cyclohexyl, R' = Me   66   7.5   :   1
(1b) R = cyclohexyl, R' = MeO   47   50   :   1

Unequivocal assignment of the relative stereochemistry of the prepared methylenecyclopropanes could in some cases be made on the basis of NMR studies and independent synthesis. However, for the more substituted methylenecyclopropanes [i.e. compounds (2b) and (3a)] single-crystal X-ray diffraction studies were necessary in order to establish the relative stereochemistries of the compounds. Compounds (2b) and (3a) are shown in Figs. 1 and 2, respectively.

(2b)   (3a)

In compound (2b) there are intermolecular hydrogen bonds between the methoxy O atoms and the hydroxyl H atoms (see Fig. 1), and infinite chains of hydrogen-bonded molecules are formed via glide-plane symmetry transformations [$O(2)\cdots O(1)(x, \frac{1}{2}-y, \frac{1}{2}+z)$ 2.862 (3) Å]. The two independent molecules in the asymmetric unit of compound (3a) are linked by O—H$\cdots$O hydrogen bonds between hydroxyl groups and with an inversion-symmetry-related pair

Fig. 2. A view of a hydrogen-bonded tetramer of compound (3a) with the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 25% probability level. Hydroxyl H atoms are drawn as spheres of arbitrary radii and the H atoms bonded to C atoms have been omitted.

form a centrosymmetric tetramer as shown in Fig. 2 [$O(1A)\cdots O(1B)$ 2.782 (4) and $O(1A)\cdots O(1B)(1-x, -y, 2-z)$ 2.835 (4) Å].

The two independent molecules in compound (3a) are essentially identical, apart from the positions of the hydroxyl H atoms. The torsion angle H(1)—O(1)—C(6)—C(1) is −122 (4)° in molecule A and −64 (5)° in molecule B. This angular difference is necessary for the molecules to form the linear O—H$\cdots$O arrangement required for the hydrogen-bonding mode present.

The geometry of the cyclopropane ring is similar in the two title compounds and the bonds adjacent to the methylene group are shorter than the bond opposite it in both cases. The average cyclopropane ring distances are C(1)—C(2) 1.534 (9), C(1)—C(3) 1.458 (3) and C(2)—C(3) 1.454 (6) Å. The changes in the geometry of a cyclopropane ring caused by the addition of a methylene group have been highlighted in the structure determination of 3-methylene-trans-1,2-cyclopropanedicarboxylic acid (Ramasubbu & Venkatesan, 1982).
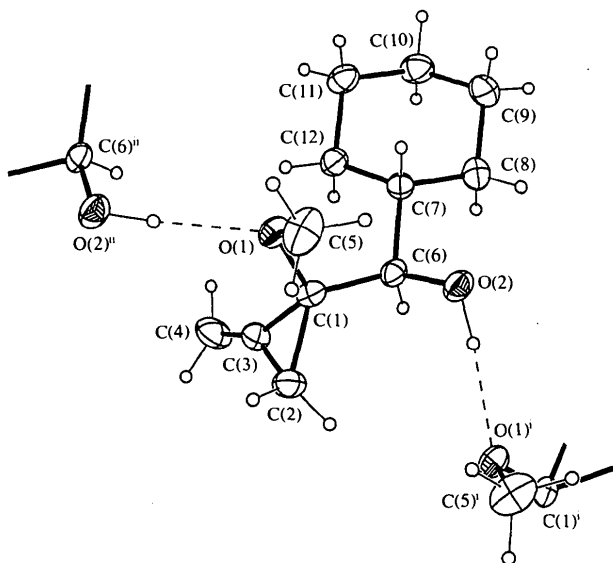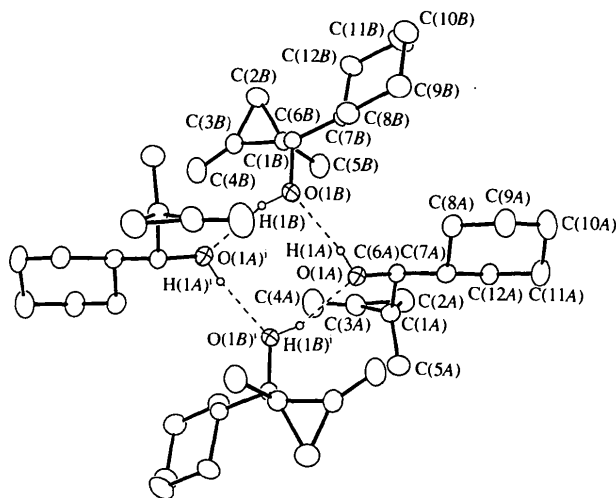
Experimental

Compound (2b)

Crystal data

Fig. 1. A view of compound (2b) with the crystallographic numbering scheme showing the hydrogen bonds to neighbouring molecules. Displacement ellipsoids are drawn at the 25% probability level and H atoms are drawn as spheres of arbitrary radii.

$C_{12}H_{20}O_2$	Mo $K\alpha$ radiation
$M_r = 196.3$	$\lambda = 0.71073$ Å
Monoclinic	Cell parameters from 25
$P2_1/c$	reflections
$a = 12.398$ (2) Å	$\theta = 20.3–27.7°$
$b = 10.057$ (1) Å	$\mu = 0.072$ mm^{-1}
$c = 10.177$ (1) Å	$T = 293$ (2) K
$\beta = 109.65$ (1)°	Needle
$V = 1194.9$ (5) Å^3	0.25 × 0.23 × 0.17 mm

$Z = 4$
$D_x = 1.091$ Mg m^{-3}

Colourless
Crystal source: diethyl ether

Data collection

Enraf–Nonius CAD-4 diffractometer	$\theta_{max} = 25.0°$
ω–2θ scans	$h = 0 \rightarrow 14$
Absorption correction:	$k = -11 \rightarrow 7$
none	$l = -12 \rightarrow 11$
2512 measured reflections	3 standard reflections
2294 independent reflections	frequency: 120 min
1308 observed reflections	intensity decay: linear
$[I > 2\sigma(I)]$	correction for 51%
$R_{int} = 0.0275$	intensity decay

Refinement

Refinement on F	$\Delta\rho_{max} = 0.20$ e Å^{-3}
$R = 0.0511$	$\Delta\rho_{min} = -0.17$ e Å^{-3}
$wR = 0.0799$	Atomic scattering factors
$S = 1.17$	from *International Tables*
1308 reflections	*for Crystallography* (1992,
132 parameters	Vol. C, Tables 4.2.6.8 and
$w = 1/[\sigma^2(F) + 0.0034F^2]$	6.1.1.4)
$(\Delta/\sigma)_{max} = 0.02$	

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (2b)

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

	x	y	z	U_{eq}
O(1)	0.9029 (2)	0.2365 (2)	0.5143 (2)	0.047 (1)
O(2)	0.8935 (2)	0.0961 (2)	0.7834 (2)	0.054 (1)
C(1)	0.8347 (2)	0.2623 (2)	0.5989 (2)	0.041 (1)
C(2)	0.8545 (3)	0.3947 (2)	0.6761 (3)	0.057 (1)
C(3)	0.7544 (3)	0.3725 (2)	0.5520 (3)	0.050 (1)
C(4)	0.6589 (3)	0.4163 (3)	0.4622 (4)	0.075 (1)
C(5)	1.0208 (3)	0.2132 (4)	0.5894 (3)	0.078 (2)
C(6)	0.8010 (2)	0.1422 (2)	0.6659 (2)	0.042 (1)
C(7)	0.7599 (2)	0.0249 (2)	0.5662 (2)	0.042 (1)
C(8)	0.7112 (3)	−0.0860 (3)	0.6328 (3)	0.057 (1)
C(9)	0.6759 (3)	−0.2072 (3)	0.5375 (3)	0.068 (1)
C(10)	0.5921 (3)	−0.1703 (3)	0.3952 (3)	0.066 (1)
C(11)	0.6386 (3)	−0.0585 (3)	0.3300 (3)	0.059 (1)
C(12)	0.6721 (2)	0.0622 (3)	0.4265 (2)	0.047 (1)

Table 2. *Selected geometric parameters* (Å, °) *and hydrogen-bonding geometry* (Å, °) *for* (2b)

O(1)—C(1)	1.418 (4)	C(1)—C(6)	1.514 (4)
O(1)—C(5)	1.422 (3)	C(2)—C(3)	1.460 (3)
O(2)—C(6)	1.427 (3)	C(3)—C(4)	1.305 (4)
C(1)—C(2)	1.523 (3)	C(6)—C(7)	1.527 (3)
C(1)—C(3)	1.459 (4)		

C(1)—O(1)—C(5)	114.8 (2)	C(1)—C(3)—C(2)	62.9 (2)
O(1)—C(1)—C(2)	116.6 (2)	C(1)—C(3)—C(4)	147.6 (3)
O(1)—C(1)—C(3)	115.0 (2)	C(2)—C(3)—C(4)	149.5 (3)
C(2)—C(1)—C(3)	58.6 (2)	O(2)—C(6)—C(1)	111.8 (2)
O(1)—C(1)—C(6)	116.0 (2)	O(2)—C(6)—C(7)	107.5 (2)
C(2)—C(1)—C(6)	119.1 (2)	C(1)—C(6)—C(7)	113.5 (2)
C(3)—C(1)—C(6)	119.5 (2)	C(6)—C(7)—C(8)	111.2 (2)
C(1)—C(2)—C(3)	58.5 (2)	C(6)—C(7)—C(12)	113.9 (2)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O(2)—H(2)$\cdots$O(1^i)	0.95 (4)	1.91 (4)	2.862 (3)	173 (3)

Symmetry code: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$.

Compound (3a)

Crystal data

$C_{12}H_{20}O$	Mo $K\alpha$ radiation
$M_r = 180.3$	$\lambda = 0.71073$ Å
Monoclinic	Cell parameters from 25
$P2_1/c$	reflections
$a = 11.290$ (2) Å	$\theta = 20.5$–$36.1°$
$b = 19.433$ (2) Å	$\mu = 0.064$ mm^{-1}
$c = 11.782$ (2) Å	$T = 293$ (2) K
$\beta = 118.22$ (2)°	Block
$V = 2277.7$ (6) Å^3	0.50 × 0.40 × 0.35 mm
$Z = 8$	Colourless
$D_x = 1.051$ Mg m^{-3}	Crystal source: diethyl ether

Data collection

Enraf–Nonius CAD-4 diffractometer	$\theta_{max} = 26.4°$
ω scans	$h = 0 \rightarrow 14$
Absorption correction:	$k = -24 \rightarrow 0$
none	$l = -14 \rightarrow 11$
4603 measured reflections	3 standard reflections
4412 independent reflections	frequency: 120 min
1528 observed reflections	intensity decay: linear
$[I > 3\sigma(I)]$	correction for 77%
$R_{int} = 0.0171$	intensity decay

Refinement

Refinement on F	$\Delta\rho_{max} = 0.16$ e Å^{-3}
$R = 0.0515$	$\Delta\rho_{min} = -0.22$ e Å^{-3}
$wR = 0.0610$	Atomic scattering factors
$S = 1.35$	from *International Tables*
1528 reflections	*for Crystallography* (1992,
244 parameters	Vol. C, Tables 4.2.6.8 and
$w = 1/[\sigma^2(F) + 0.0010F^2]$	6.1.1.4)
$(\Delta/\sigma)_{max} = 0.26$	

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (3a)

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

	x	y	z	U_{eq}
O(1A)	0.6186 (3)	0.0664 (1)	0.9595 (2)	0.057 (1)
C(1A)	0.6871 (4)	0.0343 (2)	0.8035 (3)	0.053 (1)
C(2A)	0.6346 (5)	0.0303 (2)	0.6575 (3)	0.078 (1)
C(3A)	0.5892 (4)	−0.0170 (2)	0.7235 (4)	0.068 (1)
C(4A)	0.5146 (5)	−0.0684 (2)	0.7176 (4)	0.093 (1)
C(5A)	0.8286 (4)	0.0091 (2)	0.8896 (4)	0.073 (1)
C(6A)	0.6367 (3)	0.0919 (2)	0.8544 (3)	0.046 (1)
C(7A)	0.7265 (4)	0.1551 (2)	0.8994 (3)	0.048 (1)
C(8A)	0.6641 (4)	0.2122 (2)	0.9418 (3)	0.056 (1)
C(9A)	0.7492 (4)	0.2765 (2)	0.9835 (3)	0.070 (1)
C(10A)	0.7800 (4)	0.3027 (2)	0.8799 (4)	0.074 (1)
C(11A)	0.8468 (4)	0.2473 (2)	0.8398 (3)	0.067 (1)
C(12A)	0.7601 (4)	0.1828 (2)	0.7961 (3)	0.056 (1)
O(1B)	0.3599 (3)	0.0662 (1)	0.9321 (2)	0.053 (1)
C(1B)	0.1640 (4)	0.0632 (2)	0.7225 (3)	0.049 (1)
C(2B)	0.0088 (4)	0.0638 (2)	0.6554 (4)	0.071 (1)
C(3B)	0.0859 (4)	0.0026 (2)	0.7193 (3)	0.055 (1)
C(4B)	0.0869 (5)	−0.0614 (2)	0.7515 (3)	0.074 (1)
C(5B)	0.2312 (4)	0.0636 (2)	0.6387 (3)	0.071 (1)
C(6B)	0.2356 (3)	0.1002 (2)	0.8500 (3)	0.046 (1)
C(7B)	0.2707 (3)	0.1752 (2)	0.8436 (3)	0.044 (1)
C(8B)	0.3313 (4)	0.2087 (2)	0.9771 (3)	0.060 (1)

C(9B)	0.3605 (4)	0.2848 (2)	0.9754 (3)	0.067 (1)
C(10B)	0.2390 (4)	0.3240 (2)	0.8792 (3)	0.070 (1)
C(11B)	0.1847 (5)	0.2927 (2)	0.7477 (3)	0.073 (1)
C(12B)	0.1503 (4)	0.2169 (2)	0.7479 (3)	0.059 (1)

Table 4. *Selected geometric parameters* (Å, °) *and hydrogen-bonding geometry* (Å, °) *for* (3a)

O(1A)—C(6A)	1.435 (5)	O(1B)—C(6B)	1.434 (4)
C(1A)—C(2A)	1.534 (5)	C(1B)—C(2B)	1.544 (6)
C(1A)—C(3A)	1.455 (5)	C(1B)—C(3B)	1.461 (6)
C(1A)—C(5A)	1.512 (5)	C(1B)—C(5B)	1.503 (7)
C(1A)—C(6A)	1.504 (6)	C(1B)—C(6B)	1.509 (4)
C(2A)—C(3A)	1.445 (7)	C(2B)—C(3B)	1.456 (5)
C(3A)—C(4A)	1.287 (7)	C(3B)—C(4B)	1.297 (5)
C(6A)—C(7A)	1.519 (5)	C(6B)—C(7B)	1.523 (5)
C(2A)—C(1A)—C(3A)	57.8 (3)	C(2B)—C(1B)—C(3B)	57.9 (2)
C(2A)—C(1A)—C(5A)	117.5 (4)	C(2B)—C(1B)—C(5B)	117.8 (3)
C(3A)—C(1A)—C(5A)	116.8 (3)	C(3B)—C(1B)—C(5B)	118.3 (3)
C(2A)—C(1A)—C(6A)	117.8 (3)	C(2B)—C(1B)—C(6B)	116.7 (4)
C(3A)—C(1A)—C(6A)	116.9 (4)	C(3B)—C(1B)—C(6B)	116.2 (3)
C(5A)—C(1A)—C(6A)	116.9 (3)	C(5B)—C(1B)—C(6B)	116.9 (3)
C(1A)—C(2A)—C(3A)	58.4 (3)	C(1B)—C(2B)—C(3B)	58.2 (2)
C(1A)—C(3A)—C(2A)	63.8 (3)	C(1B)—C(3B)—C(2B)	63.9 (3)
C(1A)—C(3A)—C(4A)	147.5 (4)	C(1B)—C(3B)—C(4B)	147.4 (4)
C(2A)—C(4A)—C(4A)	148.6 (4)	C(2B)—C(3B)—C(4B)	148.7 (4)
O(1A)—C(6A)—C(1A)	108.8 (3)	O(1B)—C(6B)—C(1B)	110.2 (3)
O(1A)—C(6A)—C(7A)	108.8 (3)	O(1B)—C(6B)—C(7B)	106.2 (3)
C(1A)—C(6A)—C(7A)	115.1 (4)	C(1B)—C(6B)—C(7B)	115.9 (3)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
(O1A)—H(1A)⋯O(1B)	0.77 (5)	1.98 (5)	2.782 (4)	171 (4)
(O1B)—H(1B)⋯O(1A^i)	0.81 (5)	2.01 (4)	2.835 (4)	157 (4)

Symmetry code: (i) $1 - x, -y, 2 - z$.

Each crystal suffered from significant linear intensity decay which was corrected for accordingly. H atoms bonded to C atoms were included in the refinement in calculated positions (C—H 0.96 Å) and treated as riding atoms. The hydroxyl H atoms were refined with isotropic displacement parameters.

For both compounds, data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD-4 Software* (Siemens, 1993); program(s) used to solve structures: *SHELXTL/PC XS* (Sheldrick, 1990); program(s) used to refine structures: *SHELXTL/PC XLS3*; molecular graphics: *SHELXTL/PC XP*; software used to prepare material for publication: *SHELXTL/PC XPUBL*.

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3,7-Dinitronoradamantane, $C_9H_{12}N_2O_4$, and 3,7,9-Trinitronoradamantane, $C_9H_{11}N_3O_6$

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Abstract

The possible C_{2v} molecular symmetry for the dinitronoradamantane compound is not present; however, the carbon cages in each of the title compounds [3a,6a-dinitrooctahydro-2,5-methanopentalene and 3a,6a,7-trinitrooctahydro-2,5-methanopentalene, respectively] have approximate C_{2v} symmetry. Although the C—C—N—O torsion angles of the nitro groups differ significantly from the 90° required for C_{2v} molecular symmetry, approximate C_2 symmetry is maintained for both molecules in the asymmetric unit. Bond distances and angles are near expected values with the exception of the C3—C7 bond distance in both title compounds which averages 1.594 (4) Å.

Comment

Polynitropolycyclic cage molecules are of interest because of their possible use as high-energy density materials (Marchand, 1988) and polynitroadamantanes are compounds of this class for which there has been