Table 3. *Torsion angles* (°) *about the exocyclic chain*

C(9)–S–C(8)–C(7)	132·5 (4)	N–C(2)–C(7)–C(8)	4·4 (6)
C(10)–S–C(8)–C(7)	−121·4 (4)	N–C(2)–C(7)–C(71)	−115·1 (5)
S–C(8)–C(7)–C(2)	−60·6 (5)	N–C(2)–C(7)–C(72)	122·0 (5)
S–C(8)–C(7)–C(71)	60·2 (5)	C(3)–C(2)–C(7)–C(71)	64·6 (7)
S–C(8)–C(7)–C(72)	178·2 (4)	C(3)–C(2)–C(7)–C(72)	−58·3 (7)

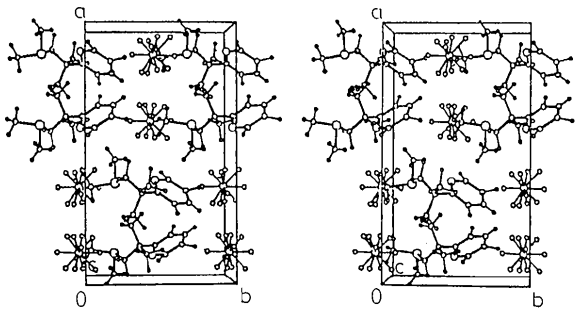

Fig. 2. Stereoscopic view of the crystal structure.

interaction between S and N. It is interesting that the weak S···N interaction has been found for such an open chain system which is able to rotate around the single bonds, C(2)–C(7) and C(7)–C(8).

Fig. 2 shows the molecular packing viewed along the *b* axis. There is no special intermolecular contact shorter than the van der Waals contact.

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Acta Cryst. (1987). C**43**, 2340–2343

Structure of 1-(2-Hydroxyethyl)-3,4-bis(trimethylsilyl)-8-oxabicyclo[4.3.0]nonadien-6-ol

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Abstract. $C_{16}H_{30}O_3Si_2$, $M_r = 326{\cdot}59$, triclinic, $P\bar{1}$, $a = 6{\cdot}857$ (1), $b = 10{\cdot}090$ (1), $c = 14{\cdot}477$ (2) Å, $\alpha = 81{\cdot}54$ (1), $\beta = 89{\cdot}51$ (1), $\gamma = 73{\cdot}71$ (1)°, $V = 950{\cdot}4$ (3) Å^3, $Z = 2$, $D_m = 1{\cdot}12$, $D_x = 1{\cdot}141$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 1{\cdot}873$ cm^{-1}, $F(000) = 356$, $T = 298$ K, $R = 0{\cdot}036$, $wR = 0{\cdot}048$, 1940 observed reflections [$I \geq 3\sigma(I)$]. The steric crowding caused by the vicinal trimethylsilyl groups distorts the six-membered ring as compared with unsubstituted 1,3-cyclohexadiene. Each molecule is hydrogen-bonded to one translationally related neighbor *via* the hydroxyl groups. The resulting chains are in turn hydrogen-bonded to one neighboring chain by means of two symmetrically equivalent hydrogen bonds between pairs of molecules. The double chains thus formed are oriented along the *a* axis, the direction of most rapid growth of the crystal.

Introduction. The title compound was prepared by D. Harvey and K. P. C. Vollhardt of this department as part of an ongoing investigation of [2+2+2] cycloadditions mediated by $(\eta^5\text{-}C_5H_5)Co(CO)_2$. The reaction involved furyl propargyl ether and bis(trimethylsilyl)-ethyne in the presence of $(\eta^5\text{-}C_5H_5)Co(CO)_2$, sub-

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sequent hydrolysis, oxidative decomplexation of the $(\eta^5\text{-}C_5H_5)Co$ moiety and reduction of the product (Harvey & Vollhardt, 1987). An X-ray crystallographic structure determination was undertaken after analysis of spectroscopic data failed to establish unambiguously the structure of the reaction product.

Experimental. Colorless crystals provided by D. Harvey of this department. D_m measured by flotation in an aqueous solution of KI. Sample crystal was a parallelepiped of dimensions $0{\cdot}10 \times 0{\cdot}13 \times 0{\cdot}55$ mm. Enraf–Nonius CAD-4 diffractometer; 24 reflections ($27{\cdot}0 \le 2\theta \le 29{\cdot}0°$) used to refine cell parameters. Data collection: $3 \le 2\theta \le 45°$, index ranges $0 \le h \le 7$, $-10 \le k \le 10$, $-15 \le l \le 15$; θ–2θ scan technique with Mo $K\alpha_2$ ($\lambda = 0{\cdot}71073$ Å) at room temperature, max./min. scan speed: $6{\cdot}7/0{\cdot}74°$ min^{-1}. 2732 total reflections; rejections: $(0kl)$, $k < 0$; $(00l)$, $l < 0$ (redundant data); 2480 unique reflections; 1940 reflections with $(F_o)^2 \ge 3\sigma(F_o)^2$. No indication of crystal decomposition from three standard reflections measured every 2 h. No absorption correction needed, ψ-scan variation ±3% in I. Structure solved by direct methods (*MULTAN*) and refined *via* standard full-matrix least squares and Fourier techniques with a Digital Equipment Corporation μ-VAX computer using locally modified Nonius *SDP* software (Frenz, 1985). Function minimized was $\sum w(|F_o| - |F_c|)^2$, $w = 1/\sigma^2(F_o)$, $\sigma(F_o^2) = [\sigma_0^2(F_o^2) + (pF_o^2)^2]^{1/2}$; $p = 0{\cdot}03$; non-hydrogen atoms refined anisotropically. H atoms located on difference map, positions of H atoms bound to C atoms calculated using idealized geometry and C–H distance of 0·95 Å, but not refined; isotropic thermal parameters assigned by $B(\text{H}) = 1{\cdot}3 \times B_{eq}(\text{C})$. Hydroxyl H atoms were located on a difference map and refined isotropically. Final number of parameters refined = 199, $R = 0{\cdot}0362$, $wR = 0{\cdot}0484$, $S = 2{\cdot}250$, max. shift/e.s.d. in final cycle 0·01; largest peak on final difference Fourier map = 0·24 e Å^{-3}; secondary-extinction coefficient = $8{\cdot}5\ (2) \times 10^{-7}$ (Zachariasen, 1963), included and refined. Atomic scattering factors and anomalous corrections from *International Tables for X-ray Crystallography* (1974).

Discussion. A drawing of the title compound with the atom-numbering scheme is shown in Fig. 1. Atomic coordinates and final equivalent isotropic thermal parameters of all non-hydrogen atoms are given in Table 1. Table 2 lists selected interatomic distances and angles.*

The steric crowding caused by the vicinal trimethylsilyl groups has several effects on the molecular structure. Bond angles and distances of the six-membered ring are significantly different from those in 1,3-cyclohexadiene (Oberhammer & Bauer, 1969) or *transoid*-1,3-butadiene (Almenningen, Bastiansen & Trætteberg, 1958), as determined by gas electron diffraction. The C(4)–C(3) bond is longer [1·511 (2) Å] than in the unsubstituted ring [1·47 (1) Å] or the straight-chain diene [1·48 (1) Å]. The Si(2)–C(4)–C(3) and Si(1)–C(3)–C(4) bond angles are on average 7·5° larger than the corresponding H–C–C angles in 1,3-cyclohexadiene; the other angles around C(4) and C(3) are therefore smaller. The consequence of a longer C(4)–C(3) bond and smaller ring angles around these atoms is also noticeable at C(2) and C(5), which have larger ring angles of 126·0 (2) and 123·9 (2)°, respectively, compared with the value of 120·1 (5)° for the unsubstituted ring (Oberhammer & Bauer, 1969). Whereas the torsion angle C(5)–C(4)–C(3)–C(2), 17·3 (3)°, is nearly the same as in 1,3-cyclohexadiene, the torsion angle Si(2)–C(4)–C(3)–Si(1) is 34·1 (3)° and is affected by steric interactions. There are also deformations in the trimethylsilyl groups caused by steric interactions between the methyl group C(15) and C(16) on Si(2) and C(13) and C(14) on Si(1). The distances are 3·710 (4) Å for C(15)–C(13), 3·616 (3) Å for C(15)–C(14) and 3·680 (4) Å for C(16)–C(13). The C(4)–Si(2)–C(15) and C(3)–Si(1)–C(13) bond angles, 115·7 (1) and 113·8 (1)°, respectively, are significantly larger than the average of the other angles around Si(2) and Si(1), 108·2 (1) and 108·6 (1)°, respectively.

Another interesting feature of the crystal structure is the hydrogen-bonding network. The β-hydroxyethyl chain of each molecule is extended towards the hydrogen atom of O(1) of the translationally related molecule in the next unit cell. The intermolecular O(1)–O(2) distance is 2·748 (2) Å, which is within the

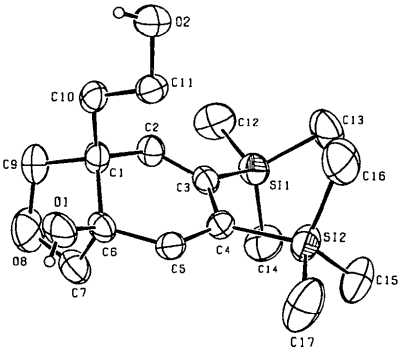

Fig. 1. *ORTEP* drawing (Johnson, 1976) of the title compound showing the atomic numbering scheme. Ellipsoids are drawn at the 50% probability level.

* Lists of structure factors, anisotropic thermal parameters, least-squares-planes data, torsion and intramolecular angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44212 (25 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates and final equivalent isotropic thermal parameters*

	x	y	z	B_{eq}(Å^2)
Si(1)	0·2650 (1)	0·7394 (1)	0·5898 (1)	3·73 (2)
Si(2)	0·1856 (1)	0·4815 (1)	0·7967 (1)	3·93 (2)
O(1)	−0·2531 (2)	0·9111 (2)	0·9159 (1)	3·80 (4)
O(2)	0·3944 (3)	0·8637 (2)	0·9854 (1)	4·22 (4)
O(8)	−0·3590 (3)	1·0904 (2)	0·7292 (2)	5·99 (6)
C(1)	−0·0306 (4)	0·9696 (2)	0·7973 (2)	2·76 (5)
C(2)	0·0917 (4)	0·9105 (2)	0·7181 (2)	2·90 (5)
C(3)	0·1344 (3)	0·7781 (2)	0·7018 (2)	2·73 (5)
C(4)	0·0592 (4)	0·6764 (2)	0·7699 (2)	2·74 (5)
C(5)	−0·0876 (3)	0·7303 (2)	0·8265 (2)	2·85 (5)
C(6)	−0·1803 (3)	0·8837 (2)	0·8254 (2)	2·82 (5)
C(7)	−0·3462 (4)	0·9472 (3)	0·7500 (2)	4·13 (7)
C(9)	−0·1784 (4)	1·1134 (3)	0·7616 (2)	4·17 (7)
C(10)	0·1114 (4)	0·9814 (2)	0·8750 (2)	3·03 (5)
C(11)	0·2432 (4)	0·8445 (2)	0·9255 (2)	3·16 (5)
C(12)	0·3086 (5)	0·9018 (3)	0·5248 (2)	5·74 (8)
C(13)	0·5221 (5)	0·6102 (4)	0·6077 (3)	6·44 (9)
C(14)	0·0920 (5)	0·6834 (3)	0·5152 (2)	5·52 (8)
C(15)	0·1986 (6)	0·3833 (3)	0·6969 (2)	6·05 (9)
C(16)	0·4432 (5)	0·4592 (4)	0·8474 (3)	7·1 (1)
C(17)	0·0400 (6)	0·4000 (3)	0·8861 (3)	6·7 (1)

The thermal parameter given for anisotropically refined atoms is the isotropic equivalent thermal parameter defined as $\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$, where a,b,c are real cell parameters and $B(i,j)$ are anisotropic betas. Numbers in parentheses are the estimated standard deviations of the last digits of the given values.

Table 2. *Selected interatomic distances* (Å), *bond angles* (°) *and torsion angles* (°)

Si(2)–C(4)	1·895 (2)	Si(2)–C(15)	1·856 (2)
Si(2)–C(16)	1·860 (2)	Si(2)–C(17)	1·864 (3)
Si(1)–C(3)	1·884 (2)	Si(1)–C(12)	1·865 (2)
Si(1)–C(13)	1·868 (2)	Si(1)–C(14)	1·864 (2)
C(4)–C(3)	1·511 (2)	C(3)–C(2)	1·341 (2)
C(2)–C(1)	1·510 (2)	C(1)–C(6)	1·536 (2)
C(6)–C(5)	1·496 (2)	C(5)–C(4)	1·339 (2)
C(1)–C(9)	1·537 (2)	C(9)–O(8)	1·419 (2)
O(8)–C(7)	1·409 (2)	C(7)–C(6)	1·517 (2)
C(1)–C(10)	1·533 (2)	C(10)–C(11)	1·507 (2)
C(11)–O(2)	1·429 (2)	C(6)–O(1)	1·435 (2)
O(2)–O(1^{i})	2·748 (2)	O(1)–O(2^{ii})	2·801 (2)
O(1)–H(O2^{ii})	2·091 (1)	O(2)–H(O1^{i})	2·079 (1)

C(4)–Si(2)–C(15)	115·7 (1)	C(4)–Si(2)–C(16)	106·8 (1)
C(4)–Si(2)–C(17)	109·7 (1)	C(15)–Si(2)–C(16)	111·4 (1)
C(15)–Si(2)–C(17)	104·9 (1)	C(16)–Si(2)–C(17)	108·3 (1)
C(3)–Si(1)–C(12)	109·7 (1)	C(3)–Si(1)–C(13)	113·8 (1)
C(3)–Si(1)–C(14)	108·3 (1)	C(12)–Si(1)–C(13)	105·3 (1)
C(12)–Si(1)–C(14)	107·3 (1)	C(13)–Si(1)–C(14)	112·2 (1)
C(3)–C(4)–C(5)	117·1 (1)	Si(2)–C(4)–C(3)	125·2 (1)
Si(2)–C(4)–C(5)	116·7 (1)	C(4)–C(3)–C(2)	117·7 (2)
C(4)–C(3)–Si(1)	125·6 (1)	Si(1)–C(3)–C(2)	116·4 (1)
C(1)–C(10)–C(11)	115·4 (1)	C(10)–C(11)–O(2)	112·1 (1)
C(2)–C(1)–C(6)	108·0 (1)	C(2)–C(1)–C(9)	110·3 (1)
C(2)–C(1)–C(10)	110·2 (1)	C(6)–C(1)–C(9)	100·9 (1)
C(6)–C(1)–C(10)	116·8 (1)	C(9)–C(1)–C(10)	110·3 (1)
C(1)–C(6)–C(5)	112·9 (1)	C(1)–C(6)–C(7)	101·0 (1)
C(1)–C(6)–O(1)	108·0 (1)	C(5)–C(6)–C(7)	112·8 (1)
C(5)–C(6)–O(1)	110·4 (1)	C(7)–C(6)–O(1)	111·3 (1)
O(1)–H(O2^{ii})–O(2^{ii})	162·9 (1)	O(2)–H(O1^{i})–O(1^{i})	169·9 (1)

Si(1)–C(3)–C(4)–Si(2)	34·1 (3)	C(2)–C(3)–C(4)–C(5)	17·3 (3)
C(2)–C(1)–C(6)–C(5)	41·0 (3)	C(9)–C(1)–C(6)–C(7)	36·0 (2)
Si(1)–C(3)–C(2)–C(1)	173·3 (2)	Si(2)–C(4)–C(5)–C(6)	169·9 (2)

Symmetry codes: (i) $-x, y, z$; (ii) $-x, 2-y, 2-z$.

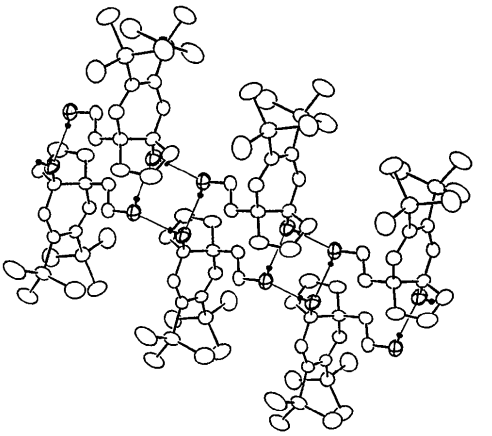

Fig. 2. *ORTEP* drawing (Johnson, 1976) showing the hydrogen-bonding network. The chains drawn are oriented along the *a* axis. Hydrogen bonds are drawn as thin lines.

range of 2·70–2·90 Å reported for hydrogen-bonded hydroxyl compounds in the literature (Wells, 1986); the O(1)–H(O1)–O(2) angle is 169·6 (1)°. Each O(1) atom is itself hydrogen-bonded to H(O2) of a molecule related by $-x, 2-y, 2-z$ to the base molecule. H(O2) of the base molecule is in turn hydrogen-bonded to O(1) of the same neighbor in a symmetric fashion. These equivalent hydrogen bonds exhibit an O(1)–O(2) distance of 2·801 (2) Å and an O(1)–H(O2)–O(2) angle of 163·4 (1)° and serve as cross links between two endless chains of molecules connected by the other set of hydrogen bonds. This is illustrated in Fig. 2. The direction of these double chains is along the crystallographic *a* axis, which is the direction of fastest growth of the crystal. To our knowledge, this structure determination is the first of a compound of the type described. Further ramifications of this compound and its synthesis will be discussed elsewhere (Harvey & Vollhardt, 1987).

This crystal structure was solved at the X-ray Crystallographic Facility (CHEXRAY) at the Department of Chemistry, University of California, Berkeley, as part of the requirements of a graduate chemistry course on structure analysis by X-ray diffraction. We thank a referee for helpful comments and Mr P. Smith, Dr F. Hollander and Professor K. N. Raymond for their guidance. WCAW acknowledges a Geneviève Lichtig fellowship from the University of California.

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Captodative Substitution and Cyclopropane Geometry. VI. Structure of Dimethyl *cis*-1,2-Bis(phenylthio)-1,2-cyclopropanedicarboxylate

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Abstract. $C_{19}H_{18}O_4S_2$, $M_r = 374{\cdot}48$, monoclinic, $P2_1/a$, $a = 8{\cdot}159\ (5)$, $b = 21{\cdot}093\ (17)$, $c = 11{\cdot}153\ (11)$ Å, $\beta = 105{\cdot}63\ (6)°$, $V = 1848\ (3)$ Å^3, $Z = 4$, $D_x = 1{\cdot}35$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 3{\cdot}05$ cm^{-1}, $F(000) = 784$, $T = 291$ K, $R = 0{\cdot}038$ for 1975 observed reflections. One of the methoxycarbonyl groups bisects the cyclopropyl ring while the other adopts the less favorable perpendicular conformation. The effects of the substituents on the ring bond lengths are clearly dependent on the orientation of the π-acceptor groups: in the bisecting position they shorten the distal bond while, when perpendicular, the effects are negligible. The values of the distal-bond shortenings observed for the S—*R* and COOMe groups agree very well with literature data.

Introduction. In the course of our work on polar-substituent effects on cyclopropane geometry (Tinant, Wu, Declercq, Van Meerssche, De Mesmaeker, Masamba, Merenyi & Viehe, 1985, 1987), we have determined the X-ray structure of the title compound. This derivative was chosen because it is the only one in the series of bis(captodative)-substituted cyclopropanes for which the *cis* isomer was more stable than the *trans* isomer (Masamba, 1986). Moreover, the *cis* configuration of the methoxycarbonyl groups should force each one to adopt a different orientation towards the cyclopropyl ring. It offers thus the opportunity to estimate the effect of the orientation of the π-acceptor group on the ring bond-length pattern.

Experimental. Crystals obtained by evaporation from ether–petroleum ether. D_m not measured. Parallelepiped crystal with dimensions 0·15 × 0·18 × 0·3 mm. Lattice parameters refined using 15 reflections in the range $5 \le 2\theta \le 25°$. Syntex $P2_1$ diffractometer, graphite-monochromatized Mo $K\alpha$ radiation. 2737 $hk\pm l$ independent reflections with $(\sin\theta)/\lambda \le 0{\cdot}561$ Å^{-1}; $0 \le h \le 9, 0 \le k \le 23, -12 \le l \le 12$; 1975 with $I \ge 2{\cdot}5\sigma(I)$. Standard reflection 401 checked every 50 reflections: no significant deviation. Structure solved by *SHELXS*86 (Sheldrick, 1985). H atoms from difference Fourier synthesis. Anisotropic least-squares refinement (*SHELX*76, Sheldrick, 1976) using F; H isotropic with common refined temperature factor. $w = 1/(\sigma^2 + 0{\cdot}00067F^2)$. $R = 0{\cdot}038$, $wR = 0{\cdot}041$ for 1975 observed reflections. Final maximum shift to e.s.d. = 0·31 (y of C7). $S = 1{\cdot}28$. Maximum and minimum heights in final difference Fourier synthesis = 0·21 and −0·20 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. The atomic parameters are given in Table 1.* Fig. 1 is a stereoscopic view of the molecule, showing the numbering of the atoms (program *PLUTO*, Motherwell & Clegg, 1978). Bond distances and angles are given in Table 2. As a consequence of the steric conflict resulting from their *cis* configuration, the two methoxycarbonyl groups adopt a completely different orientation towards the cyclopropyl ring. The torsion angles *M*23—C1—C4—O5 = −76° and *M*13—C2—C8—O9 = 2° (*M*13 and *M*23 being respectively the midpoints of the C1—C3 and C2—C3 bonds), indicate that the methoxycarbonyl at C1 is in the perpendicular position while that at C2 adopts the preferred *s-cis* bisected orientation (Korp, Bernal & Fuchs, 1983). The phenyl groups of the two thiophenyl substituents are perpendicular to each other (dihedral angle between

* 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 44222 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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