1985), 1-acetoxyrubescensine A (Chen, Lin, Zhang & Li, 1983) and trichorabdal F acetate (Kashyap, Watson, Grossie, Node, Sai, Fujita & Fuji, 1984), it is found that these compounds all possess a 2-methylene-cyclopentanone fragment, the structural data of which are quite similar. In addition, this fragment of ganervosin B is located on the side of molecule with no steric hindrance (see Fig. 1), so it would react with other compounds more easily. This compound, therefore, would be expected to have anti-tumor activity.

Fig. 2. gives the packing view in a unit cell. The principal bond lengths and bond angles in ganervosin B are shown in Table 2.

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Structure of Methyl (E)-p-[3,3,3-Trifluoro-2-(2,2,4,4-tetramethyl-6-thiochromanyl)-1-propenyl]benzoate

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Abstract. Methyl (E)-p-[3,3,3-trifluoro-2-(2,2,4,4-tetramethyl-6-thiochromanyl)-1-propenyl]benzoate, $C_{24}H_{25}F_3O_2S$, $M_r = 434.52$, monoclinic, $P2_1/n$, $a = 16.475$ (9), $b = 16.519$ (6), $c = 8.024$ (4) Å, $\beta = 101.84$ (5)°, $V = 2137.27$ Å^3, $Z = 4$, $D_x = 1.35$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 1.52$ cm^{-1}, $F(000) = 912$, $T = 138$ (2) K, $R = 0.035$ for 3869 data. The configuration about the C(11)–C(13) double bond is such that the thiochromanyl group and the benzoate group are *cis* to each other. The sulfur-containing ring is closer to a half-chair than a sofa conformation. The conformations and bond distances of nine differently substituted thiochromans are discussed. It is concluded that the difference in S—C(sp^2) and S—C(sp^3) distances occurs when the sulfur atom is not substituted but that this difference is not present when the ring is oxidized to a sulfone.

Introduction. Retinoids (vitamin A and derivatives thereof), arotinoids (molecules with an aryl ring fused to the saturated ring of a retinoid) and heteroarotinoids (molecules with a heteroatom in the saturated ring of an arotinoid) are of current interest in anticancer-drug design (Waugh, Berlin, Ford, Holt, Carrol, Schomber, Thompson & Schiff, 1985). Many of these compounds have the ability to inhibit the induction of epidermal ornithine decarboxylase (ODC) by the tumor promotor 12-O-tetradecanoylphorbol-13-acetate (TPA). Moreover, toxicity studies have indicated that hetero-arotinoids are less toxic than the retinoids and the arotinoids (Dawson, Hobbs, Derdzinshki, Chan, Gruber, Chao, Smith, Thies & Schiff, 1984; Metra, Schiff, Moore, Buckley & Dawson, 1986). The hetero-arotinoid ethyl (E)-p-[2-(4,4-dimethyl-6-thiochromanyl)propenyl]benzoate, (I), has been synthesized and

Table 1. *Final coordinates and isotropic equivalent thermal parameters of non-hydrogen atoms with e.s.d.'s in parentheses*

	x	y	z	U_{eq}*
S(1)	0·53821 (2)	0·41163 (2)	−0·33029 (5)	0·0301 (1)
C(2)	0·62675 (9)	0·46796 (8)	−0·2118 (2)	0·0247 (5)
C(3)	0·68558 (9)	0·40797 (9)	−0·1035 (2)	0·0240 (5)
C(4)	0·65583 (9)	0·35866 (9)	0·0357 (2)	0·0239 (5)
C(4a)	0·56706 (9)	0·32726 (8)	−0·0194 (2)	0·0192 (4)
C(5)	0·53749 (9)	0·27344 (8)	0·0889 (2)	0·0203 (4)
C(6)	0·45802 (8)	0·24140 (8)	0·0530 (2)	0·0196 (4)
C(7)	0·40415 (9)	0·26591 (9)	−0·0967 (2)	0·0225 (5)
C(8)	0·43146 (9)	0·31856 (9)	−0·2062 (2)	0·0234 (5)
C(8a)	0·51220 (9)	0·34916 (8)	−0·1710 (2)	0·0202 (4)
C(9)	0·66367 (13)	0·40742 (12)	0·2020 (2)	0·0390 (6)
C(10)	0·71568 (10)	0·28611 (11)	0·0750 (2)	0·0349 (6)
C(11)	0·42991 (9)	0·18305 (8)	0·1709 (2)	0·0205 (4)
C(12)	0·42676 (9)	0·21705 (9)	0·3426 (2)	0·0232 (4)
C(13)	0·40677 (9)	0·10599 (8)	0·1392 (2)	0·0216 (4)
C(14)	0·40220 (9)	0·05689 (8)	−0·0159 (2)	0·0210 (4)
C(15)	0·35793 (9)	−0·01560 (9)	−0·0229 (2)	0·0240 (5)
C(16)	0·34576 (9)	−0·06474 (9)	−0·1654 (2)	0·0248 (5)
C(17)	0·37939 (9)	−0·04316 (8)	−0·3045 (2)	0·0222 (4)
C(18)	0·42731 (9)	0·02663 (9)	−0·2953 (2)	0·0248 (5)
C(19)	0·43862 (10)	0·07604 (9)	−0·1534 (2)	0·0239 (5)
C(20)	0·36493 (9)	−0·09163 (9)	−0·4641 (2)	0·0263 (5)
C(21)	0·66899 (11)	0·50386 (10)	−0·3475 (2)	0·0306 (5)
C(22)	0·59769 (13)	0·53616 (11)	−0·1105 (3)	0·0408 (7)
F(23)	0·50156 (6)	0·23548 (7)	0·4344 (1)	0·0474 (4)
F(24)	0·39246 (7)	0·16800 (5)	0·4404 (1)	0·0406 (4)
F(25)	0·38314 (6)	0·28583 (5)	0·3312 (1)	0·0396 (3)
O(26)	0·38393 (8)	−0·07055 (7)	−0·5950 (1)	0·0387 (4)
O(27)	0·32703 (7)	−0·16225 (6)	−0·4476 (1)	0·0320 (4)
C(28)	0·30996 (14)	−0·21283 (12)	−0·5982 (2)	0·0395 (6)

$$* \ U_{eq} = \tfrac{1}{3}\sum_i\sum_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j \ (\text{Å}^2).$$

the crystal structure has been determined (Waugh *et al.*, 1985).

(I)
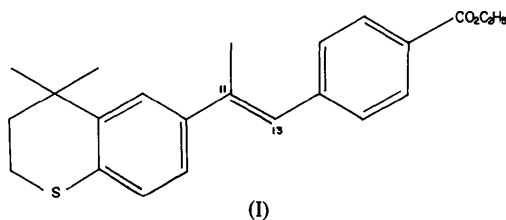
In the structure of compound (I), the geometric arrangement of the C(11)—C(13) double bond [corresponding to the C(9)—C(10) double bond in retinoic acid, (II)] is important for the antitumor activity of the compound (Dawson, Hobbs, Chan, Chao & Fung, 1981).

(II)
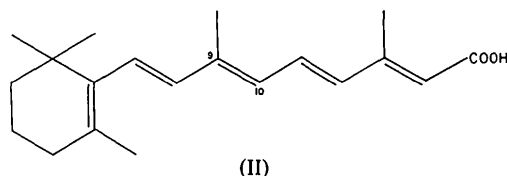
The methyl (*E*)-*p*-[3,3,3-trifluoro-2-(2,2,4,4-tetramethyl-6-thiochromanyl)-1-propenyl]benzoate, compound (III), is one of eleven new heteroarotinoids of

which the synthesis and biological activity will be published (Spruce, Berlin, Verma, Breitman, Ji & van der Helm, 1989). It is also a representative of six trifluoromethyl-substituted heteroarotinoids which are of interest for two reasons. First, due to the electronegativity of fluorine at the allylic carbon [*i.e.* C(12)], the electronic environments of nearby atoms will be altered without an appreciable change in spatial requirement when compared to the nonfluorinated molecule. Also, fluorine can be used as a ^{19}F NMR biological probe and utilization of fluorine in this manner might lead to information on the mechanism by which these heteroarotinoids affect cell differentiation. Compound (III) is similar to compound (I), but differs from compound (I), mainly, by the substitution of a trifluoromethyl group for a methyl group on C(11). Using ^{19}F NMR analysis, a tentative stereochemical assignment was made for compound (III) with the thiochromanyl group and the benzoate group *cis* to each other (Spruce *et al.*, 1989). The single-crystal X-ray analysis of compound (III) was carried out and confirmed the tentative assignment based on ^{19}F NMR studies.

(III)
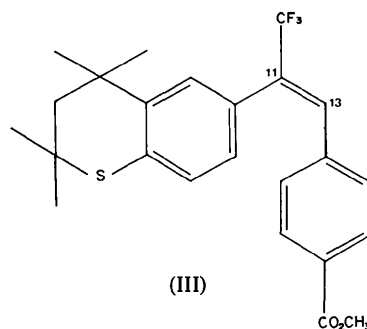
Experimental. A crystal of dimensions 0·31 × 0·37 × 0·52 mm, was used for the X-ray data collection on an Enraf–Nonius CAD-4 at T = 138 (2) K. Because of the light and heat sensitivity of the crystal, the crystal mounting was carried out with grease in a low-temperature N_2 current (~150 K), and the data collection was carried out in the dark. 72 reflections with $10 < \theta < 15°$ were used for the lattice constants. Systematic absences were $0k0$ ($k = 2n + 1$), $h0l$ ($h + l = 2n + 1$). All data with $1·0 \le 2\theta \le 53·0°$, and $-20 \le h \le 20$, $0 \le k \le 20$, $0 \le l \le 10$ were collected using a θ–2θ scan technique and a variable scan width calculated as $(0·90 + 0·20\tan\theta)°$. The maximum scan time was 60 s with 40 s used for scanning the peak and 10 s used for scanning each of the left and right backgrounds. The receiving aperture, located 173 mm from the data crystal, had a variable width, which was calculated as $(3·50 + 0·86\tan\theta)$ mm, while the height of the aperture remained constant at 6 mm. Three intensity control monitors were measured every 2 h of X-ray exposure time which showed a maximum difference of

$$C_{24}H_{25}F_3O_2S$$

0·026 and an e.s.d. of 0·008. The profiles of all reflections were observed and stored. The data set was processed using Blessing's (1987) profile analysis method and program. Monochromator and Lorentz–polarization corrections were applied. No absorption correction was made. Among 4734 unique reflections there were 865 unobserved data $[I \leq 2\sigma(I)]$. The position of the sulfur atom in the asymmetric unit was obtained by using the heavy-atom method. The structure was completed and refined with the program *SHELX*76 (Sheldrick, 1976) utilizing 3869 data, and anisotropic temperature factors for non-hydrogen atoms. The locations of all the hydrogen atoms were determined from successive difference Fourier syntheses and refined isotropically. A final R of 0·035 and wR of 0·041 were obtained by the minimization of $\sum w(|F_o| - |kF_c|)^2$ with $w = 1/\sigma^2(F)$. The maximum shift/e.s.d. was 0·060 for non-hydrogen atoms and 0·068 for hydrogen atoms. The maximum electron density in the final difference Fourier map was 0·28 e Å^{-3} and the minimum was −0·27 e Å^{-3}. The 'error of fit' function $[\sum w(F_o - F_c)^2/(N - Np)]^{1/2}$ was 2·5. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).*

Discussion. The final coordinates of the non-hydrogen atoms are given in Table 1. A stereoview (Johnson, 1965) and the atom-numbering scheme of a single molecule are shown in Fig. 1. Bond distances, angles and selected torsion angles are presented in Table 2.

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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 51565 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

S(1)–C(2)	1·824 (1)	C(11)–C(12)	1·498 (2)
S(1)–C(8a)	1·763 (1)	C(11)–C(13)	1·338 (2)
C(2)–C(3)	1·527 (2)	C(12)–F(23)	1·335 (2)
C(2)–C(21)	1·528 (2)	C(12)–F(24)	1·332 (2)
C(2)–C(22)	1·523 (2)	C(12)–F(25)	1·337 (2)
C(3)–C(4)	1·541 (2)	C(13)–C(14)	1·474 (2)
C(4)–C(4a)	1·529 (2)	C(14)–C(15)	1·397 (2)
C(4)–C(9)	1·541 (2)	C(14)–C(19)	1·396 (2)
C(4)–C(10)	1·543 (2)	C(15)–C(16)	1·383 (2)
C(4a)–C(5)	1·399 (2)	C(16)–C(17)	1·391 (2)
C(4a)–C(8a)	1·406 (2)	C(17)–C(18)	1·391 (2)
C(5)–C(6)	1·387 (2)	C(17)–C(20)	1·487 (2)
C(6)–C(7)	1·399 (2)	C(18)–C(19)	1·382 (2)
C(6)–C(11)	1·490 (2)	C(20)–O(26)	1·207 (2)
C(7)–C(8)	1·376 (2)	C(20)–O(27)	1·343 (2)
C(8)–C(8a)	1·397 (2)	O(27)–C(28)	1·448 (2)

S(1)–C(2)–C(3)	108·18 (9)	C(9)–C(4)–C(10)	107·0 (1)
S(1)–C(2)–C(21)	105·00 (9)	C(11)–C(12)–F(23)	113·0 (1)
S(1)–C(2)–C(22)	110·5 (1)	C(11)–C(12)–F(24)	114·4 (1)
S(1)–C(8a)–C(8)	115·37 (9)	C(11)–C(12)–F(25)	112·0 (1)
S(1)–C(8a)–C(4a)	124·7 (1)	C(11)–C(13)–C(14)	130·3 (1)
C(2)–S(1)–C(8a)	102·00 (6)	C(11)–C(13)–H(13)	117·3 (8)
C(2)–C(3)–C(4)	119·8 (1)	C(12)–C(11)–C(13)	118·0 (1)
C(3)–C(2)–C(21)	109·2 (1)	C(13)–C(14)–C(15)	116·2 (1)
C(3)–C(2)–C(22)	114·1 (1)	C(13)–C(14)–C(19)	125·9 (1)
C(3)–C(4)–C(4a)	113·4 (1)	C(14)–C(13)–H(13)	112·3 (8)
C(3)–C(4)–C(9)	111·6 (1)	C(14)–C(15)–C(16)	121·5 (1)
C(3)–C(4)–C(10)	105·9 (1)	C(14)–C(19)–C(18)	120·7 (1)
C(4)–C(4a)–C(5)	118·1 (1)	C(15)–C(14)–C(19)	117·9 (1)
C(4)–C(4a)–C(8a)	124·7 (1)	C(15)–C(16)–C(17)	119·9 (1)
C(4a)–C(4)–C(9)	109·4 (1)	C(16)–C(17)–C(18)	119·0 (1)
C(4a)–C(4)–C(10)	109·2 (1)	C(16)–C(17)–C(20)	122·2 (1)
C(4a)–C(5)–C(6)	123·2 (1)	C(17)–C(18)–C(19)	120·9 (1)
C(4a)–C(8a)–C(8)	119·9 (1)	C(17)–C(20)–O(26)	124·7 (1)
C(5)–C(4a)–C(8a)	117·2 (1)	C(17)–C(20)–O(27)	112·2 (1)
C(5)–C(6)–C(7)	118·3 (1)	C(18)–C(17)–C(20)	118·8 (1)
C(5)–C(6)–C(11)	121·2 (1)	C(20)–O(27)–C(28)	115·7 (1)
C(6)–C(7)–C(8)	119·9 (1)	C(21)–C(2)–C(22)	109·4 (1)
C(6)–C(11)–C(12)	114·6 (1)	F(23)–C(12)–F(24)	105·6 (1)
C(6)–C(11)–C(13)	127·4 (1)	F(23)–C(12)–F(25)	105·4 (1)
C(7)–C(6)–C(11)	120·5 (1)	F(24)–C(12)–F(25)	105·7 (1)
C(7)–C(8)–C(8a)	121·5 (1)	O(26)–C(20)–O(27)	123·1 (1)

C(5)–C(6)–C(11)–C(13)	−116·9 (2)	C(15)–C(14)–C(13)–C(11)	−165·8 (1)

The structure determination shows that the thiochromanyl group and the benzoate group are *cis* to each other with respect to the C(11)–C(13) double bond, confirming the stereochemical assignment made by ^{19}F NMR spectroscopy (Spruce *et al.*, 1989).

The CF$_3$ substitution of the double bond has interesting effects on several conformational features of the molecule. The atom C(6) is forced to assume a staggered conformation with respect to the bulky CF$_3$ group, giving a *gauche* conformation of C(6) with F(23) and F(25). The third fluorine atom F(24), therefore, lies in the plane of the double bond yielding a short contact with the allylic hydrogen atom, H(13). This contact distance is 2·27 Å and is significantly less than the sum of the van der Waals radii of the F and H atoms (2·55 Å). One can consider this a weak hydrogen bond or, more likely, an electrostatic interaction. A very similar interaction has been observed in (*E*)-α-(trifluoromethyl)stilbene (Ruban, Zobel, Kossmann & Nuck, 1980) under identical conditions.
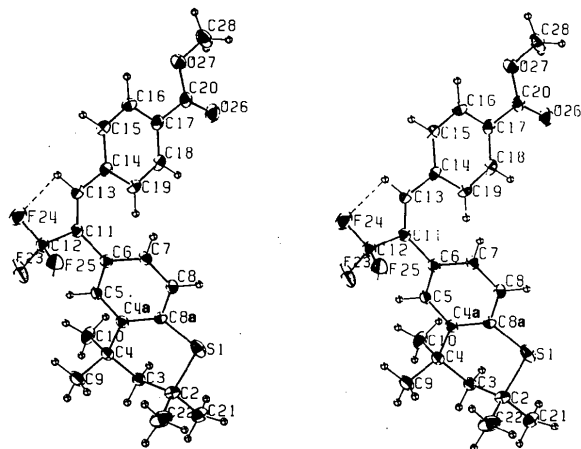

Fig. 1. The stereoview of a single molecule and atom-numbering scheme of methyl (*E*)-*p*-[3,3,3-trifluoro-2-(2,2,4,4-tetramethyl-6-thiochromanyl)-1-propenyl]benzoate.

Table 3. *Selected structural parameters of the heterocyclic ring in the thiochroman ring system*

Compound	(a)	(b)	(c)	(d)	(e)	(f)	(g)	(h)	(i)
Bond lengths (Å)									
S(1)—C(2)	1·824 (1)	1·766	1·800	1·778 1·786	1·818	1·818	1·761	1·761	1·843
S(1)—C(8a)	1·763 (1)	1·763	1·759	1·761 1·759	1·770	1·712	1·760	1·767	1·762
Asymmetry parameters									
$\Delta C_s(2)$	14·1	9·2	35·1	15·7 31·9	27·6	24·8	16·4	20·8	72·6
$\Delta C_s(3)$	27·3	34·9	11·2	22·9 15·2	23·1	12·7	25·1	22·6	51·1
$\Delta C_2(2–3)$	10·8	18·6	16·5	5·9 11·9	3·5	6·7	6·6	3·2	87·4
$\Delta C_s(2–3)$	—	—	—	—	—	—	—	—	28·2
$\Delta C_s(1)$	—	—	—	—	—	—	—	—	21·5
Conformation	2,3-half-chair	2-sofa	3-sofa	2,3-half-chair	2,3-half-chair	2,3-half-chair	2,3-half-chair	2,3-half-chair	boat twisted

This orientation of the CF_3 group in turn determines the conformation of the C(6)—C(11) bond. Coplanarity of the aromatic ring [C(4a)—C(8a)] and the double bond is not possible because it would yield a contact between H(5) and F(23) and F(25) which is too small. Instead the aromatic ring is turned around the C(6)—C(11) bond by 63° such that the contact distance between F(23) and H(5) (2·49 Å) is close to the sum of the van der Waals radii (2·55 Å, Pauling, 1960) [C(13)—C(11)—C(6)—C(5) is −116·9°].

The conformation about the C(14)—C(13) bond is correlated with the conformation of the C(6)—C(11) bond and the tendency of the benzoate group to be coplanar with the double bond. The aromatic ring has to be turned away from the double-bond plane in order to remove an unfavorable contact of 1·5 Å between C(7) and H(19) which would exist when the torsional angle around C(13)—C(14) was 180°. The ring is rotated by 14° yielding a contact distance between C(7) and H(19) of 2·71 Å, somewhat less than the sum of the van der Waals radii (2·90 Å). A very similar conformation for the aromatic rings is found in (E)-α-(trifluoromethyl)stilbene (Ruban *et al.*, 1980).

The conformation of the sulfur-containing ring is between a half-chair and a sofa. The asymmetry parameters (Duax & Norton, 1975) are $\Delta C_2(2–3)$ = 10·8 (for an ideal half-chair conformation $\Delta C_2 = 0$) and $\Delta C_s(2) = 14\cdot1$ (for an ideal sofa $\Delta C_s = 0$). This indicates that compound (III) is closer to a half-chair conformation. The asymmetry parameters and the structures of compound (III) and several other 'half-chair', 'sofa' and 'boat' conformers are compared in Table 3. The structures of the thiochroman ring systems of these thiochroman derivatives are shown in Fig. 2. From the comparison shown in Fig. 2, one cannot easily deduce a fundamental reason for the heterocyclic ring to assume a particular conformation. Compound (f) (half-chair) and compound (i) (boat) differ from each other only by a methyl group at
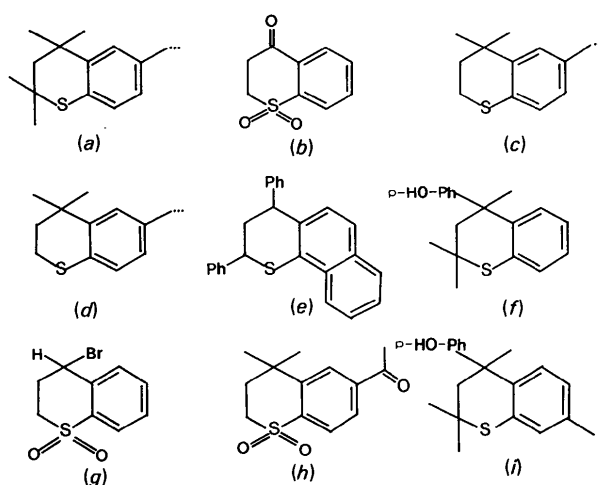

Fig. 2. The thiochroman ring systems in related structures. [(a), (d)–(h): half-chair; (b), (c): sofa; (i): boat]. (a) Methyl (E)-p-[3,3,3-trifluoro-2-(2,2,4,4-tetramethyl-6-thiochromanyl)-1-propenyl]benzoate [compound (III), present work]. (b) Thiochroman-4-one 1,1-dioxide (Ealick, van der Helm, Baker & Berlin, 1979). (c) [3-(4,4-Dimethyl-6-thiochromanyl)-2-butenyl]triphenylphosphonium bromide (Hossain, van der Helm & Berlin, 1987). (d) Ethyl (E)-p-[2-(4,4-dimethyl-6-thiochromanyl)propenyl]benzoate [compound (I), Waugh *et al.*, 1985]. (e) 2,4-Diphenyl-7,8-benzo-2,3-dihydrothiochroman (Kharchenko, Kriven'ko, Fedotova, Evtushenko, Shcherbakov, Aleksandrov & Struchkov, 1980). (f) 4-p-Hydroxyphenyl-2,2,4-trimethylthiochroman (McNicol, Mills & Wilson, 1969). (g) 4-Bromothiochroman 1,1-dioxide (Andreetti, Bocelli & Sgarabotto, 1978). (h) 4,4-Dimethyl-6-thiochromanyl methyl ketone 1,1-dioxide (Waugh *et al.*, 1985). (i) 4-p-Hydroxyphenyl-2,2,4,7-tetramethylthiochroman (Hardy, McKendrick & McNicol, 1977).

position C(7). Compound (c) (sofa) and compound (d) (half-chair), however, have the same substitution pattern.

The C—S bonds involving the sp^3-hybridized C(2) and the sp^2-hybridized C(8a) have nearly equal lengths in the sulfones (b), (g) and (h) but are significantly

different in all other compounds (Table 3). The inequality of the lengths of $S-C(sp^2)$ and $S-C(sp^3)$ is easily understood and is due to a difference in hybridization of the carbon atoms. The approximate equality of these two bonds in the sulfones is possibly correlated with the electron-withdrawing effect of the oxygen atoms.

The molecular packing in the crystal is due to van der Waals forces. The shortest intermolecular distance is 2·31 Å between H(22)b and H'(22)b $(-x, -y, -z)$.

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Structures of Monoethanolamine (MEAM), Diethanolamine (DEAM) and Triethanolamine (TEAM)

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Abstract. MEAM: 2-aminoethanol, C_2H_7NO, $M_r = 61·08$, monoclinic, Cc, $a = 5·026$ (3), $b = 8·818$ (6), $c = 8·319$ (7) Å, $\beta = 107·44$ (6)°, $V = 351·74$ Å^3, $Z = 4$, $D_x = 1·15$ Mg m^{-3}, $\lambda(Mo\ K\bar{\alpha}) = 0·71069$ Å, $\mu = 0·085$ mm^{-1}, $F(000) = 136$, $T = 263$ K, $R = 0·044$ for 494 unique observed reflections. DEAM: 2,2'-iminodiethanol, $C_4H_{11}NO_2$, $M_r = 105·14$, monoclinic, $P2_1/c$, $a = 4·464$ (1), $b = 13·052$ (2), $c = 9·812$ (2) Å, $\beta = 93·73$ (2)°, $V = 570·47$ Å^3, $Z = 4$, $D_x = 1·22$ Mg m^{-3}, $\lambda(Mo\ K\bar{\alpha}) = 0·71069$ Å, $\mu = 0·090$ mm^{-1}, $F(000) = 232$, $T = 192$ K, $R = 0·030$ for 921 unique observed reflections. TEAM: 2,2',2''-nitrilotriethanol, $C_6H_{15}NO_3$, $M_r = 149·19$, rhombohedral, $R\bar{3}$, $a = 11·491$ (1), $c = 10·070$ (1) Å {the c-axis length was incorrectly given in a preliminary report of the TEAM structure [Brodalla & Mootz (1981). *Angew. Chem.* 93, 824; *Angew. Chem. Int. Ed. Engl.* 20, 791–792]}, $V = 1151·53$ Å^3, $Z = 6$, $D_x = 1·29$ Mg m^{-3}, $\lambda(Mo\ K\bar{\alpha}) = 0·71069$ Å, $\mu = 0·095$ mm^{-1}, $F(000) = 492$, $T = 140$ K, $R = 0·033$ for 721 unique observed reflections. The crystal structures are governed by the geometry of the molecules and extensive intermolecular hydrogen bonding. The MEAM molecules are arranged in a three-dimensional network with strong $N-H\cdots O$ as well as weak $N-H\cdots O$ and $O-H\cdots N$ bonds. Rings of two $O-H\cdots O$-bridged DEAM molecules are linked *via* strong $O-H\cdots N$ bonds into one-dimensional tube-like stacks; weak $N-H\cdots O$ bonds across the rings are also present. The TEAM molecules are linked to form discrete cage-like dimers with point symmetry $\bar{3}$ *via* rings of six strong $O-H\cdots O$ bonds with chair conformation.

Introduction. In the course of our investigations of hydrogen-bonded solids we have determined the crystal structures of the ethanolamines MEAM, DEAM and