Table 2. *Hydrogen-bond parameters with e.s.d.'s in parentheses*

X—H···Y	d(H···Y) (Å)	d(X···Y) (Å)	$\angle$(X—H···Y) (°)
N(10)—H(10*a*)···N(1^{i})	2·16 (5)	2·995 (6)	176 (4)
N(10)—H(10*b*)···O(1^{ii})	2·16 (5)	3·063 (6)	159 (4)
O(1)—H(11*w*)···N(7^{ii})	2·02 (7)	2·856 (5)	161 (7)
O(1)—H(12*w*)···O(2^{iii})	2·28 (7)	2·804 (5)	146 (8)
O(2)—H(21*w*)···O(1^{iii})	2·33 (7)	2·804 (5)	144 (9)
O(2)—H(22*w*)···N(3^{ii})	1·85 (7)	2·848 (5)	176 (6)

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

hydrogen bonds between water molecules in adjacent layers. The cyclic water dimer formed in this way (Table 2) exhibits a shortened transannular H···H van der Waals contact of 1·86 Å. Hydrogen bonding between water molecules is thus expected to be rather weak.

The crystal packing found in 8-ethyl-9-methyladenine dihydrate may explain the decomposition of the crystals in air at room temperature. The presence of holes along the *ab* planes filled by weakly bound water molecules facilitates diffusion of the latter to the crystal surface.

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Structure of the Zwitterionic 10-[2-(2-Dimethylsulfonioethoxy)ethoxy]undecahydro-7,8-dicarba-*nido*-undecaborate(1−)

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Abstract. $C_8H_{25}B_9O_2S$, $M_r = 282\cdot64$, orthorhombic, $P2_12_12_1$, $a = 8\cdot799$ (3), $b = 11\cdot268$ (3), $c = 16\cdot012$ (4) Å, $V = 1587\cdot5$ (2) Å^3, $Z = 4$, $D_m = 1\cdot180$, $D_x = 1\cdot183$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0\cdot184$ mm^{-1}, $F(000) = 600$, $T = 293$ K, $R = 0\cdot037$ for 1910 observed independent reflections. The O—C—C—O—C—C (derived from opening of a dioxane ring) is bound to the *nido* eleven-vertex carbaborane cage which has negative charge [B—O = 1·420 (3) Å], and to the $S(CH_3)_2$ group (positive charge [C—S = 1·803 (2) Å]. In the carbaborane cage, mean B—B = 1·774 (3), mean C—B = 1·672 (3) Å and the C—C bond is 1·536 (4) Å.

Introduction. Crystals of the title zwitterionic compound were prepared in the Institute of Inorganic Chemistry of the Czechoslovak Academy of Sciences as part of a study of carbaborane derivatives which are being screened for chemotherapeutic activity. The compound represents a whole new class, generally accessible by opening of a dioxane ring bound to the skeletal B atom by a dative bond. The reaction of 7,8-$C_2B_9H_{13}$ in the dioxane solution (373 K, 20 hours) with Lewis base $(CH_3)_2S$ opens the dioxane ring producing $(CH_3)_2S$—$CH_2CH_2OCH_2CH_2O$—7,8-$C_2B_9H_{11}$ (Plešek, Štíbr & Heřmánek, 1989). Other β-dialkyl ether derivatives show the same behaviour.

Experimental. Transparent colourless crystal 0·3 × 0·3 × 0·5 mm; D_m by flotation; Hilger & Watts diffractometer; Mo $K\alpha$ radiation, Nb filter; cell parameters and standard deviations by least squares from 33 reflections ($6 < \theta < 19°$) (Shoemaker, 1970); 1997 unique independent reflections by learnt profile method (Clegg, 1981) measured by $\theta/2\theta$ scans to $\sin\theta/\lambda = 0\cdot6387$ Å^{-1} for $h = 0$–10, $k = 0$–13, $l = 0$–20. 1910 reflections with $I > 1\cdot96\sigma(I)$ regarded as observed. Intensities of three standards (400, 008, 051) measured every 30 reflections, no significant

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Table 1. *Fractional coordinates and* B_{eq} *values (Hamilton,* 1959) *with e.s.d.'s in parentheses, for non*-H *atoms*

$B_{eq} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}(Å^2)
S	0·49229 (5)	0·12286 (4)	0·51452 (3)	2·75 (1)
O(1)	0·5147 (2)	0·3317 (1)	0·61664 (9)	3·27 (3)
O(2)	0·4192 (2)	0·5261 (2)	0·51799 (9)	3·68 (4)
C(1)	0·5289 (3)	−0·0280 (2)	0·4870 (2)	3·96 (6)
C(2)	0·6486 (3)	0·1970 (2)	0·4671 (2)	4·28 (6)
C(3)	0·5402 (3)	0·1248 (2)	0·6240 (1)	3·46 (5)
C(4)	0·4740 (3)	0·2327 (2)	0·6649 (1)	3·43 (5)
C(5)	0·4650 (3)	0·4404 (2)	0·6511 (1)	3·18 (5)
C(6)	0·5044 (3)	0·5380 (2)	0·5919 (1)	3·46 (5)
B(1)	0·6483 (3)	0·5148 (2)	0·2932 (2)	3·16 (5)
B(2)	0·4692 (3)	0·5662 (3)	0·2612 (2)	3·65 (6)
B(3)	0·6304 (4)	0·6594 (3)	0·2539 (2)	3·59 (6)
B(4)	0·7461 (3)	0·6318 (2)	0·3404 (2)	3·07 (5)
B(5)	0·6558 (3)	0·5283 (2)	0·4034 (1)	2·67 (4)
B(6)	0·4807 (3)	0·4862 (2)	0·3531 (1)	2·95 (5)
C(7)	0·4654 (3)	0·7080 (2)	0·2994 (2)	3·97 (5)
C(8)	0·6156 (3)	0·7429 (2)	0·3416 (2)	3·68 (5)
B(9)	0·6422 (3)	0·6794 (2)	0·4305 (2)	3·40 (6)
B(10)	0·4779 (3)	0·5775 (2)	0·4437 (1)	2·81 (5)
B(11)	0·3660 (3)	0·6139 (2)	0·3511 (2)	3·50 (6)

Table 2. *Bond distances* (Å) *and selected torsion angles* (°)

S—C(1)	1·785 (2)	B(2)—B(11)	1·785 (4)
S—C(2)	1·779 (3)	B(3)—B(4)	1·747 (4)
S—C(3)	1·803 (2)	B(3)—C(7)	1·714 (4)
O(1)—C(4)	1·403 (2)	B(3)—C(8)	1·695 (4)
O(1)—C(5)	1·413 (3)	B(4)—B(5)	1·735 (3)
O(2)—C(6)	1·407 (2)	B(4)—C(8)	1·699 (3)
O(2)—B(10)	1·420 (3)	B(4)—B(9)	1·790 (4)
C(3)—C(4)	1·499 (3)	B(5)—B(6)	1·802 (3)
C(5)—C(6)	1·493 (3)	B(5)—B(9)	1·761 (3)
B(1)—B(2)	1·755 (4)	B(5)—B(10)	1·782 (4)
B(1)—B(3)	1·754 (4)	B(6)—B(10)	1·779 (3)
B(1)—B(4)	1·746 (4)	B(6)—B(11)	1·758 (3)
B(1)—B(5)	1·772 (4)	C(7)—C(8)	1·536 (4)
B(1)—B(6)	1·788 (4)	C(7)—B(11)	1·605 (4)
B(2)—B(3)	1·769 (5)	C(8)—B(9)	1·610 (4)
B(2)—B(6)	1·729 (4)	B(9)—B(10)	1·858 (4)
B(2)—C(7)	1·711 (4)	B(10)—B(11)	1·827 (4)

B(10)—O(2)—C(6)—C(5)	−155·8 (2)	C(5)—O(1)—C(4)—C(3)	−177·1 (2)
O(2)—C(6)—C(5)—O(1)	66·6 (3)	O(1)—C(4)—C(3)—S	−50·3 (2)
C(6)—C(5)—O(1)—C(4)	−175·9 (2)		

variation; data corrected for Lorentz and polarization effects, but not for absorption. Secondary isotropic extinction type I (Becker & Coppens, 1974), Gaussian distribution with the refined $g = 0{\cdot}63 \times 10^{-4}$.

Coordinates of S atom determined from Patterson map, Fourier synthesis based on phase from S provided positions of all remaining non-H atoms. Refinement with local version of least-squares program *ORFLS* (Busing, Martin & Levy, 1962), anisotropic temperature factors for non-H atoms; all H atoms from difference Fourier synthesis refined with isotropic temperature factor; function minimized $\sum w(|F_o| - |F_c|)^2$ with $w^{-1} = \sigma^2(|F_o|) + (0{\cdot}03|F_o|)^2$; in final cycle $R = 0{\cdot}037$, $wR = 0{\cdot}054$, $S = 1{\cdot}51$ (for observed reflections), $(\Delta/\sigma)_{\max} = 0{\cdot}02$; max. and min. peak heights in final difference Fourier synthesis: $+0{\cdot}24$ and $-0{\cdot}29$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Calculation performed on Siemens 7536 computer.

Discussion. Positional parameters are given in Table 1, bond lengths for non-H atoms and selected torsion angles in Table 2.* The molecular structure is shown in Fig. 1. Nine B atoms and two C atoms form a *nido* carbaborane cage with mean B—B = 1·774 (3), mean C—B = 1·672 (3) and C—C = 1·536 (4) Å. Deviations of the C(7)—C(8)—B(9)—B(10)—B(11) atoms from their mean plane range from 0·005 (3) to 0·034 (3) Å. Average distances to terminal H in the carbaborane cage are B—H = 1·11 (3) and C—H = 0·94 (4) Å. The H_b atom in the open part of the

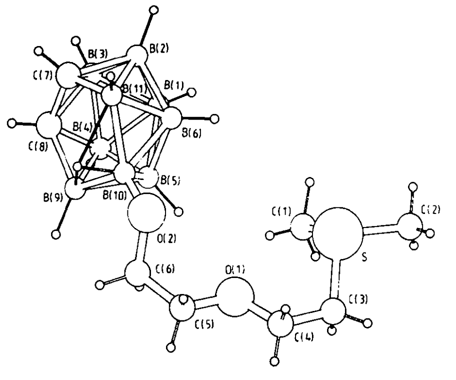

Fig. 1. Structure and numbering of the $B_9C_2H_{11}OCH_2CH_2OCH_2CH_2S(CH_3)_2$ molecule.

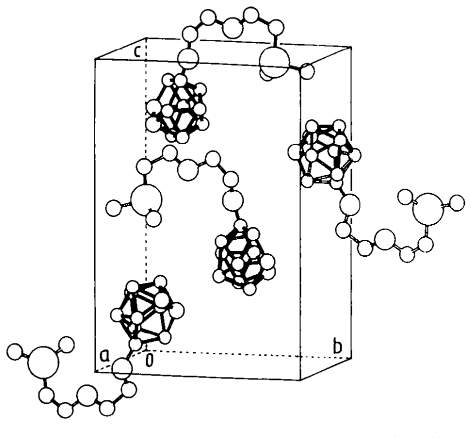

Fig 2. Packing of the molecule in the unit cell.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond distances involving H atoms and bond angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52130 (30 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

carbaborane cage forms an asymmetric bridge with $B(9)—H_b(10) = 1·12\ (3)$, $B(10)—H_b(10) = 1·49\ (4)$ and $B(11)—H_b(10) = 1·87\ (3)$ Å.

The zwitterionic compound with negative charge on the carbaborane cage and positive charge on $S(CH_3)_2$ is formed by splitting of the O—C bond of the dioxane ring, the O(2) and C(3) atoms being bonded to the carbaborane cage and to $S(CH_3)_2$, respectively. The orientation of the dioxane O(2)—C(6)—C(5)—O(1)—C(4)—C(3) chain is defined by torsion angles given in Table 2. The C—O and C—C distances in this chain, mean C—O = 1·408 (3), mean C—C = 1·496 (3) Å, are only slightly different from those reported for the dioxane ring itself: O—C = 1·425 (3), C—C = 1·478 (3) Å (Buschmann, Müller & Luger, 1986). The arrangement of the molecules in the unit cell is illustrated in Fig. 2.

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Structures de Trois Derivés de la Benzo[*f*]flavone: Fluoro-4′ Benzo[*f*]flavone, Méthoxy-4′ Benzo[*f*]flavone, Hydroxy-5 Benzo[*f*]flavone

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Abstract. BF2: $C_{19}H_{11}FO_2$, $M_r = 290·3$, monoclinic, $P2_1/n$, $a = 21·795\ (3)$, $b = 3·844\ (1)$, $c = 16·131\ (2)$ Å, $\beta = 101·31\ (2)°$, $V = 1325·2$ Å^3, $Z = 4$, $D_x = 1·456$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 8·695$ cm^{-1}, $T = 293$ K, $R = 0·052$ for 1366 observed independent reflections. BF3: $C_{20}H_{14}O_3$, $M_r = 302·3$, monoclinic, $P2_1/a$, $a = 20·633\ (3)$, $b = 3·924\ (1)$, $c = 19·537\ (3)$ Å, $\beta = 114·62\ (2)°$, $V = 1438·0$ Å^3, $Z = 4$, $D_x = 1·397$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 7·680$ cm^{-1}, $T = 293$ K, $R = 0·060$ for 1476 observed independent reflections. BF4: $C_{19}H_{12}O_3$, $M_r = 288·3$, monoclinic, $P2_1/n$, $a = 15·861\ (3)$, $b = 17·535\ (3)$, $c = 4·887\ (1)$ Å, $\beta = 95·39\ (2)°$, $V = 1353·2$ Å^3, $Z = 4$, $D_x = 1·416$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 7·886$ cm^{-1}, $T = 293$ K, $R = 0·056$ for 1321 observed independent reflections. The phenyl ring in each molecule is planar. BF4 has the least distorted fused-ring system because of hydrogen bonding between the hydroxy and carboxy groups, leading to a conjugated pseudo-ring. The benzoflavone parent molecule is more nearly planar than the substituted molecules: the phenyl ring makes an angle of 0·5° with the plane of the fused-ring system, compared with 3·3, 4·4 and 9·4° for BF2, BF3 and BF4.

Introduction. La benzo[*f*]flavone (BF1) (Rossi, Cantrell, Farber, Dyott, Carrell & Gluska, 1980) est une molécule de synthèse appartenant à la série chimique naturelle des flavones, largement représentée dans le règne végétal. La présence d'un substituant benzo l'apparente aux carbures polycycliques cancérogènes. Cette analogie se retrouve en partie dans les propriétés biologiques; BF1 est en effet un très bon inducteur enzymatique, surtout au niveau pul-

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* Décédé.

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