Table 2. *Principal bond distances* (Å) *and angles* (°) *for* (2)

O3—C3	1.454 (3)	C7—C8	1.558 (4)
O3—C16	1.336 (4)	C7—C11	1.536 (4)
O6—C6	1.451 (3)	C8—C9	1.544 (4)
O6—C18	1.342 (3)	C9—C10	1.519 (4)
O8—C8	1.457 (3)	C10—C14	1.500 (5)
O8—C20	1.336 (4)	C11—C12	1.529 (4)
O16—C16	1.200 (5)	C11—C13	1.524 (5)
O18—C18	1.203 (4)	C16—C17	1.502 (5)
O20—C20	1.209 (4)	C18—C19	1.488 (5)
C1—C2	1.517 (4)	C20—C21	1.483 (4)
C1—C10	1.327 (5)	C21—C22	1.388 (5)
C2—C3	1.535 (5)	C21—C26	1.386 (5)
C3—C4	1.509 (5)	C22—C23	1.383 (5)
C4—C5	1.342 (4)	C23—C24	1.366 (6)
C4—C15	1.496 (5)	C24—C25	1.400 (7)
C5—C6	1.497 (4)	C25—C26	1.387 (5)
C6—C7	1.541 (4)		

C3—O3—C16	117.3 (3)	C1—C10—C14	125.6 (3)
C6—O6—C18	117.3 (2)	C9—C10—C14	115.1 (3)
C8—O8—C20	118.7 (2)	C7—C11—C12	111.2 (3)
C2—C1—C10	128.5 (4)	C7—C11—C13	111.9 (2)
C1—C2—C3	107.9 (2)	C12—C11—C13	109.9 (3)
O3—C3—C2	108.5 (3)	O3—C16—O16	123.5 (3)
O3—C3—C4	108.8 (3)	O3—C16—C17	110.9 (4)
C2—C3—C4	110.8 (3)	O16—C16—C17	125.5 (4)
C3—C4—C5	117.6 (3)	O6—C18—O18	123.4 (3)
C3—C4—C15	117.2 (2)	O6—C18—C19	111.4 (3)
C5—C4—C15	124.4 (3)	O18—C18—C19	125.2 (3)
C4—C5—C6	123.6 (3)	O8—C20—O20	123.0 (3)
O6—C6—C5	109.5 (2)	O8—C20—C21	112.8 (3)
O6—C6—C7	105.8 (2)	O20—C20—C21	124.2 (3)
C5—C6—C7	112.3 (2)	C20—C21—C22	121.6 (3)
C6—C7—C8	110.3 (3)	C20—C21—C26	117.9 (3)
C6—C7—C11	112.6 (2)	C22—C21—C26	120.5 (3)
C8—C7—C11	115.3 (2)	C21—C22—C23	119.6 (4)
O8—C8—C7	109.0 (2)	C22—C23—C24	120.6 (4)
O8—C8—C9	108.0 (2)	C23—C24—C25	119.9 (4)
C7—C8—C9	116.0 (3)	C24—C25—C26	120.0 (4)
C8—C9—C10	110.5 (2)	C21—C26—C25	119.3 (4)
C1—C10—C9	119.1 (3)		

nates are presented in Table 1;* bond distances and angles are listed in Table 2. A view of the molecule is provided in Fig. 1.

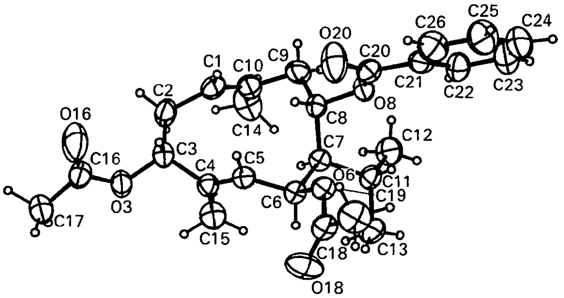

Fig. 1. *ORTEP*II (Johnson, 1976) view of (2) with non-H atoms as principal ellipses at the 50% probability level; H atoms as small spheres of arbitrary size.

Related literature. The absolute configuration of the related germacrane ester shiromodiol has been reported from its 6-*O*-acetate 8-*O*-*p*-bromobenzoate derivative (Sim, 1987). The structure of chimganidin has been determined by Makhmudov, Tashkhodzaev, Saidkhodzaev, Yagudaev & Malikov (1986).

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* Lists of structure factors, anisotropic displacement parameters, bond distances and angles involving H atoms, and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55128 (26 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST0563]

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Structure of 7-Diethylamino-4-trifluoromethylcoumarin

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Abstract. 7-Diethylamino-4-trifluoromethyl-2*H*-1-benzopyran-2-one, $C_{14}H_{14}F_3NO_2$, $M_r = 285.26$, triclinic, $P\bar{1}$, $a = 14.392$ (2), $b = 18.837$ (3), $c = 10.191$ (2) Å, $\alpha = 90.15$ (2), $\beta = 98.72$ (2), $\gamma = 85.49$ (2)°, $V = 2722.3$ (8) Å^3, $Z = 8$, $D_m = 1.405$, $D_x = 1.392$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, μ =

0108-2701/92/101859-04$06.00

1.14 cm^{-1}, $F(000) = 1184$, $T = 296$ K, final $R = 0.043$ for 3156 observed [$|F_o| \geq 5\sigma(|F_o|)$] reflections. The asymmetric unit comprises four independent molecules which can be grouped into two sets; each set contains two molecules related by a non-crystallographic centre of symmetry. These two sets are nearly orthogonal to each other. The N—C(sp^2) linkages show partial double-bond character in all molecules. The N atom and its bonded atoms are coplanar with the benzene plane and the two methyl C atoms lie on opposite sides of that plane. The N—C—C(methyl) planes are orthogonal to the benzene plane.

Experimental. Compound from Sigma Chemicals & Co., USA, green–yellow crystals from cyclohexane. A crystal of dimensions 0.4 × 0.4 × 0.2 mm was used for data collection on a Rigaku AFC-5*R* diffractometer with graphite-monochromated Mo $K\alpha$ radiation. Cell dimensions were determined from 25 reflections with 2θ angles in the range $10 \leq 2\theta \leq 20°$ and checked against oscillation and Weissenberg photographs; no mirror symmetry or systematic absences were detected in these photographs. Density, measured by flotation, showed $Z = 8$; there were no possibilities for further reduction of the cell or transformation to other systems. Intensities were measured up to $2\theta = 50°$ for $h = 0$ to 15, $k = -22$ to 22 and $l = -11$ to 11, using ω–2θ scans. Three standard reflections ($\bar{3}\bar{3}1$, $\bar{3}01$, 212) monitored every

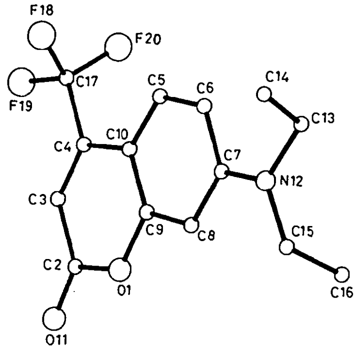

Fig. 1. Atomic numbering scheme.

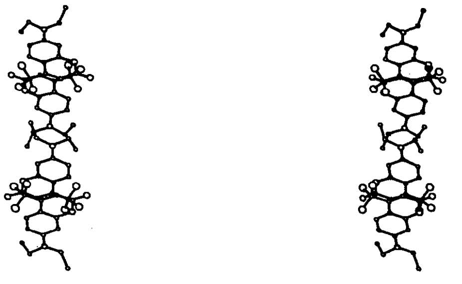

Fig. 2. Stereoview of the molecules in the asymmetric unit.

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

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Molecule (I)				
O(1)	0.3707 (2)	0.1715 (2)	−0.0021 (3)	3.8 (1)
C(2)	0.3687 (4)	0.1234 (3)	−0.1036 (5)	4.2 (2)
C(3)	0.2752 (4)	0.1076 (3)	−0.1695 (5)	4.8 (2)
C(4)	0.1963 (3)	0.1379 (3)	−0.1339 (5)	3.7 (1)
C(5)	0.1240 (3)	0.2220 (3)	0.0246 (5)	4.0 (2)
C(6)	0.1358 (3)	0.2694 (2)	0.1275 (5)	3.9 (2)
C(7)	0.2264 (3)	0.2854 (2)	0.1872 (5)	3.6 (2)
C(8)	0.3041 (3)	0.2507 (2)	0.1386 (5)	3.5 (2)
C(9)	0.2887 (3)	0.2030 (2)	0.0365 (5)	3.3 (2)
C(10)	0.2004 (3)	0.1872 (2)	−0.0274 (5)	3.2 (2)
O(11)	0.4430 (2)	0.0983 (2)	−0.1307 (4)	6.0 (1)
N(12)	0.2372 (3)	0.3327 (2)	0.2889 (4)	4.7 (2)
C(13)	0.1553 (4)	0.3730 (3)	0.3323 (5)	5.1 (2)
C(14)	0.1153 (4)	0.3343 (3)	0.4374 (6)	6.8 (2)
C(15)	0.3298 (4)	0.3530 (3)	0.3494 (5)	5.3 (2)
C(16)	0.3652 (4)	0.4117 (3)	0.2775 (5)	6.0 (2)
C(17)	0.1036 (4)	0.1217 (3)	−0.2123 (6)	5.1 (2)
F(18)	0.0459 (2)	0.0966 (2)	−0.1340 (3)	6.8 (1)
F(19)	0.1119 (2)	0.0729 (2)	−0.3041 (3)	8.2 (1)
F(20)	0.0579 (2)	0.1787 (2)	−0.2707 (3)	7.9 (1)
Molecule (II)				
O(1)	0.0986 (2)	0.0698 (2)	0.2288 (3)	4.4 (1)
C(2)	0.0932 (4)	0.1187 (3)	0.3326 (6)	5.0 (2)
C(3)	0.1806 (4)	0.1366 (3)	0.4065 (5)	4.6 (2)
C(4)	0.2640 (4)	0.1101 (3)	0.3759 (5)	4.1 (2)
C(5)	0.3511 (3)	0.0324 (3)	0.2238 (5)	4.1 (2)
C(6)	0.3467 (3)	−0.0147 (3)	0.1224 (5)	4.3 (2)
C(7)	0.2611 (3)	−0.0371 (2)	0.0557 (5)	3.7 (2)
C(8)	0.1786 (3)	−0.0063 (3)	0.0975 (5)	4.1 (2)
C(9)	0.1845 (3)	0.0423 (3)	0.1982 (5)	3.6 (2)
C(10)	0.2694 (3)	0.0625 (2)	0.2666 (5)	3.5 (2)
O(11)	0.0153 (3)	0.1412 (2)	0.3484 (4)	7.1 (2)
N(12)	0.2589 (3)	−0.0855 (2)	−0.0442 (4)	4.3 (1)
C(13)	0.3454 (3)	−0.1234 (3)	−0.0773 (5)	4.8 (2)
C(14)	0.3866 (4)	−0.0866 (3)	−0.1819 (6)	6.5 (2)
C(15)	0.1707 (4)	−0.1107 (3)	−0.1102 (5)	5.0 (2)
C(16)	0.1374 (4)	−0.1711 (3)	−0.0359 (6)	6.2 (2)
C(17)	0.3523 (4)	0.1296 (3)	0.4582 (6)	5.7 (2)
F(18)	0.4130 (2)	0.1582 (2)	0.3911 (3)	6.5 (1)
F(19)	0.3378 (2)	0.1761 (2)	0.5544 (3)	8.3 (1)
F(20)	0.4005 (2)	0.0727 (2)	0.5233 (3)	7.6 (1)
Molecule (III)				
O(1)	0.1330 (2)	0.6886 (2)	0.7486 (3)	4.0 (1)
C(2)	0.1336 (4)	0.6398 (3)	0.8487 (5)	4.5 (2)
C(3)	0.2248 (4)	0.6131 (2)	0.9173 (5)	4.3 (2)
C(4)	0.3045 (3)	0.6313 (2)	0.8805 (5)	3.8 (2)
C(5)	0.3803 (3)	0.7030 (3)	0.7193 (5)	4.0 (2)
C(6)	0.3703 (3)	0.7516 (3)	0.6195 (5)	4.4 (2)
C(7)	0.2810 (3)	0.7826 (2)	0.5595 (5)	3.7 (2)
C(8)	0.2026 (3)	0.7592 (2)	0.6106 (5)	3.6 (2)
C(9)	0.2153 (3)	0.7099 (2)	0.7102 (5)	3.3 (2)
C(10)	0.3031 (3)	0.6799 (2)	0.7715 (4)	3.2 (2)
O(11)	0.0585 (2)	0.6237 (2)	0.8730 (4)	5.9 (1)
N(12)	0.2707 (3)	0.8328 (2)	0.4613 (4)	5.0 (2)
C(13)	0.3530 (4)	0.8614 (3)	0.4143 (6)	6.0 (2)
C(14)	0.3927 (4)	0.8161 (3)	0.3103 (6)	7.0 (2)
C(15)	0.1777 (4)	0.8639 (3)	0.4013 (5)	5.6 (2)
C(16)	0.1440 (4)	0.9289 (3)	0.4712 (6)	6.8 (2)
C(17)	0.3968 (4)	0.6029 (3)	0.9564 (6)	5.3 (2)
F(18)	0.4514 (2)	0.5665 (2)	0.8802 (3)	7.3 (1)
F(19)	0.3870 (2)	0.5577 (2)	1.0520 (3)	8.6 (1)
F(20)	0.4466 (2)	0.6537 (2)	1.0113 (4)	9.4 (2)
Molecule (IV)				
O(1)	0.3932 (2)	0.5516 (2)	0.5083 (3)	4.3 (1)
C(2)	0.3982 (4)	0.6008 (3)	0.4084 (6)	4.8 (2)
C(3)	0.3087 (4)	0.6304 (3)	0.3376 (5)	4.7 (2)
C(4)	0.2262 (4)	0.6142 (3)	0.3717 (5)	4.0 (2)
C(5)	0.1432 (3)	0.5466 (3)	0.5293 (5)	4.2 (2)
C(6)	0.1480 (3)	0.4982 (3)	0.6297 (5)	4.2 (2)
C(7)	0.2350 (3)	0.4640 (2)	0.6889 (5)	3.6 (2)
C(8)	0.3162 (3)	0.4840 (3)	0.6418 (5)	3.8 (2)
C(9)	0.3081 (3)	0.5346 (2)	0.5432 (5)	3.3 (2)
C(10)	0.2231 (3)	0.5662 (2)	0.4793 (5)	3.4 (2)
O(11)	0.4747 (3)	0.6153 (2)	0.3912 (4)	6.9 (2)
N(12)	0.2402 (3)	0.4146 (2)	0.7872 (4)	4.7 (1)
C(13)	0.1561 (4)	0.3893 (3)	0.8319 (5)	5.4 (2)

Table 1 (*cont.*)

	x	y	z	B_{eq}
C(14)	0.1222 (4)	0.4348 (3)	0.9413 (5)	5.8 (2)
C(15)	0.3290 (4)	0.3765 (3)	0.8466 (5)	4.9 (2)
C(16)	0.3576 (4)	0.3129 (3)	0.7726 (5)	5.8 (2)
C(17)	0.1363 (4)	0.6449 (3)	0.2906 (6)	5.7 (2)
F(18)	0.0772 (2)	0.6789 (2)	0.3629 (3)	7.2 (1)
F(19)	0.1503 (2)	0.6907 (2)	0.1974 (3)	8.9 (1)
F(20)	0.0883 (2)	0.5936 (2)	0.2278 (3)	8.1 (1)

Table 2. *Selected bond distances* (Å), *bond angles* (°), *torsion angles* (°), *and intra- and intermolecular contacts* (Å)

	(I)	(II)	(III)	(IV)
O(1)—C(2)	1.372 (6)	1.408 (7)	1.374 (6)	1.392 (7)
O(1)—C(9)	1.389 (5)	1.382 (5)	1.390 (6)	1.387 (6)
C(2)—C(3)	1.462 (8)	1.429 (8)	1.444 (7)	1.448 (7)
C(2)—O(11)	1.205 (7)	1.201 (7)	1.206 (7)	1.193 (7)
C(3)—C(4)	1.330 (7)	1.344 (8)	1.329 (7)	1.344 (8)
C(4)—C(10)	1.424 (7)	1.436 (7)	1.438 (6)	1.431 (7)
C(4)—C(17)	1.500 (7)	1.484 (8)	1.493 (7)	1.501 (7)
C(5)—C(6)	1.375 (7)	1.358 (8)	1.354 (8)	1.362 (7)
C(5)—C(10)	1.408 (7)	1.394 (7)	1.401 (7)	1.401 (7)
C(6)—C(7)	1.408 (6)	1.409 (6)	1.418 (6)	1.412 (6)
C(7)—C(8)	1.405 (6)	1.404 (6)	1.413 (7)	1.406 (7)
C(7)—N(12)	1.364 (6)	1.363 (6)	1.362 (6)	1.359 (6)
C(8)—C(9)	1.377 (6)	1.371 (8)	1.359 (6)	1.372 (7)
C(9)—C(10)	1.391 (6)	1.392 (6)	1.399 (5)	1.386 (6)
N(12)—C(13)	1.475 (7)	1.469 (6)	1.482 (8)	1.469 (7)
N(12)—C(15)	1.460 (7)	1.457 (7)	1.462 (7)	1.462 (6)
C(13)—C(14)	1.506 (9)	1.493 (8)	1.510 (9)	1.520 (8)
C(15)—C(16)	1.492 (8)	1.516 (8)	1.499 (8)	1.478 (8)
C(17)—F(18)	1.347 (7)	1.333 (7)	1.337 (7)	1.334 (7)
C(17)—F(19)	1.322 (7)	1.342 (7)	1.326 (7)	1.333 (7)
C(17)—F(20)	1.309 (7)	1.348 (6)	1.314 (7)	1.337 (7)
C(2)—O(1)—C(9)	122.0 (4)	121.3 (4)	122.6 (4)	122.3 (4)
O(1)—C(2)—O(11)	117.9 (5)	116.1 (5)	117.6 (5)	117.4 (5)
O(1)—C(2)—C(3)	116.1 (5)	116.7 (5)	116.7 (5)	115.9 (5)
C(3)—C(2)—O(11)	126.0 (5)	127.2 (6)	125.7 (5)	126.7 (6)
C(2)—C(3)—C(4)	122.3 (5)	121.8 (5)	121.9 (5)	121.7 (5)
C(3)—C(4)—C(17)	118.6 (5)	119.2 (5)	119.5 (5)	118.7 (5)
C(3)—C(4)—C(10)	120.4 (5)	121.4 (6)	121.0 (5)	121.2 (6)
C(10)—C(4)—C(17)	120.9 (5)	119.4 (5)	119.5 (5)	120.0 (5)
C(6)—C(5)—C(10)	122.6 (5)	121.1 (5)	122.4 (5)	122.8 (5)
C(5)—C(6)—C(7)	121.1 (4)	123.0 (5)	122.6 (5)	121.3 (5)
C(6)—C(7)—N(12)	120.5 (5)	121.7 (5)	122.8 (5)	121.7 (5)
C(6)—C(7)—C(8)	117.6 (4)	116.1 (4)	115.5 (4)	116.7 (4)
C(8)—C(7)—N(12)	121.9 (5)	122.2 (5)	121.7 (5)	121.6 (5)
C(7)—C(8)—C(9)	119.2 (5)	120.0 (5)	120.3 (5)	119.9 (5)
O(1)—C(9)—C(8)	114.0 (4)	114.6 (5)	115.3 (4)	114.5 (5)
C(8)—C(9)—C(10)	124.9 (4)	123.6 (5)	124.6 (5)	124.3 (5)
O(1)—C(9)—C(10)	121.0 (4)	121.7 (5)	120.1 (4)	121.1 (4)
C(5)—C(10)—C(9)	114.5 (4)	116.2 (4)	114.6 (4)	114.9 (4)
C(4)—C(10)—C(9)	118.2 (4)	116.9 (5)	117.6 (4)	117.5 (5)
C(4)—C(10)—C(5)	127.3 (5)	126.8 (5)	127.8 (4)	127.6 (5)
C(7)—N(12)—C(15)	122.1 (4)	121.8 (5)	121.6 (5)	122.7 (5)
C(7)—N(12)—C(13)	121.4 (4)	121.8 (4)	121.9 (4)	122.6 (4)
C(13)—N(12)—C(15)	116.0 (4)	115.7 (4)	116.4 (4)	114.3 (4)
N(12)—C(13)—C(14)	112.8 (5)	113.3 (4)	113.8 (5)	112.8 (5)
N(12)—C(15)—C(16)	113.8 (5)	113.1 (5)	113.7 (5)	114.4 (5)
C(4)—C(17)—F(20)	111.8 (5)	111.8 (5)	112.3 (5)	110.9 (5)
C(4)—C(17)—F(19)	113.3 (5)	113.5 (5)	112.6 (5)	113.2 (5)
C(4)—C(17)—F(18)	111.6 (5)	114.9 (5)	112.7 (5)	113.4 (5)
F(19)—C(17)—F(20)	107.9 (5)	104.4 (5)	107.5 (5)	106.6 (5)
F(18)—C(17)—F(20)	105.8 (5)	105.8 (5)	106.1 (5)	105.5 (5)
F(18)—C(17)—F(19)	105.9 (5)	105.6 (5)	105.1 (5)	106.7 (5)
C(3)—C(4)—C(17)—F(18)	124.8 (6)	−124.6 (6)	122.1 (6)	−126.9 (6)
C(3)—C(4)—C(17)—F(19)	5.3 (8)	−2.9 (8)	3.4 (7)	−5.1 (8)
C(3)—C(4)—C(17)—F(20)	−116.9 (6)	114.8 (6)	−118.1 (6)	114.6 (6)
C(10)—C(4)—C(17)—F(18)	−58.1 (7)	56.3 (7)	−60.0 (7)	55.8 (7)
C(10)—C(4)—C(17)—F(19)	−177.5 (5)	178.0 (5)	−178.7 (4)	177.6 (5)
C(10)—C(4)—C(17)—F(20)	60.2 (7)	−64.2 (7)	59.7 (7)	−62.7 (7)
C(6)—C(7)—N(12)—C(13)	−5.2 (7)	7.5 (7)	−3.1 (8)	4.7 (8)
C(6)—C(7)—N(12)—C(15)	−177.3 (5)	177.8 (5)	−179.9 (5)	177.6 (5)
C(8)—C(7)—N(12)—C(13)	175.2 (5)	−173.0 (5)	175.4 (5)	−175.8 (5)
C(8)—C(7)—N(12)—C(15)	3.1 (7)	−2.7 (8)	−1.5 (7)	−2.9 (8)
C(7)—N(12)—C(15)—C(16)	84.6 (6)	−83.6 (6)	89.3 (6)	−84.4 (6)
C(7)—N(12)—C(13)—C(14)	89.0 (6)	−91.9 (6)	84.5 (6)	−88.4 (6)
C(13)—N(12)—C(15)—C(16)	−87.8 (6)	87.3 (6)	−87.7 (6)	89.0 (6)
C(15)—N(12)—C(13)—C(14)	−98.5 (6)	97.3 (6)	−98.5 (6)	98.2 (6)

Table 2 (*cont.*)

	(I)	(II)	(III)	(IV)
C(3)···F(19)	2.663 (6)	2.677 (6)	2.660 (6)	2.673 (6)
C(5)···F(18)	3.050 (6)	3.028 (6)	3.074 (6)	3.025 (6)
C(5)···F(20)	3.141 (6)	3.132 (6)	3.105 (6)	3.165 (6)

Short contacts between the molecules in the asymmetric unit

C(8)[I]···F(18)[II]	3.238 (5)
C(8)[II]···F(18)[I]	3.324 (6)
C(8)[III]···F(18)[IV]	3.308 (5)
C(16)[IV]···F(19)[II]	3.400 (6)

150 measurements showed no significant change. 5773 unique reflections were measured, of which 3156 were observed with $|F_o| \geq 5\sigma(|F_o|)$. Lp was corrected but not absorption; intensity data showed no systematic absences. The structure was solved by direct methods using *SHELXS*86 (Sheldrick, 1986) in the space group $P\bar{1}$. Structure solution indicated two non-crystallographic centres of symmetry in the asymmetric unit: molecules (I) and (II) were related by the inversion centre at $x = 0.238$, $y = 0.124$, $z = 0.121$ and molecules (III) and (IV) by that at $x = 0.261$, $y = 0.623$, $z = 0.625$; these positions did not change during the full-matrix least-squares refinement on F, using *SHELX*76 (Sheldrick, 1976). All H atoms were located on a difference Fourier map. Anisotropic thermal parameters were used for non-H and isotropic for H atoms; anisotropic refinement was carried out independently for each pair. Final $R = 0.043$, $wR = 0.042$, $w = 1.2318 \times [\sigma^2(|F_o|) + 0.00015F_o^2]^{-1}$, $S = 1.43$, $(\Delta/\sigma)_{\max} = 0.02$; the final difference map was featureless with maximum and minimum peak heights 0.18 and -0.19 e Å^{-3}; no correction for secondary extinction. Atomic scattering factors for all atoms were as in *SHELX*76 (Sheldrick, 1976). Geometrical calculations were performed using *PARST* (Nardelli, 1983). The atomic numbering scheme is shown in Fig. 1. The final fractional atomic coordinates and equivalent isotropic temperature factors of the non-H atoms are given in Table 1. Bond lengths, bond angles, torsion angles and intramolecular contacts involving the non-H atoms are listed in Table 2.* A stereoview of the molecules in the asymmetric unit is shown in Fig. 2.

Related literature. The title compound, a laser dye also named as coumarin 481, is found to have an exceptionally low fluorescence quantum yield in polar solvents, whereas, in non-polar solvents the

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, distances and angles involving H atoms, torsion angles, details of the least-squares plane and intermolecular distances less then 3.5 Å have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55038 (45 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: MU0286]

quantum yield is much higher (Schimitschek, Trias, Hammond & Atkins, 1974). The decrease in the fluorescence quantum yield is a result of free rotation around the N—C(sp^2) bond in the excited state and the stabilization of the non-emissive new conformer in the solvent media (Jones, Jackson & Halpern, 1980; Jones, Jackson, Choi & Bergmark, 1985; Loboda, Sokolova, Fofonova & Khochkina, 1989). The structural study, performed in order to understand the ground-state conformation of the diethylamino group, shows that any rotation about the N—C(sp^2) bond is facilitated since the methyl C atoms lie on either sides of the coumarin moiety. The structural details of related aminocoumarin dyes have been published elsewhere (Messager & Delugeard, 1974; Chinnakali, Sivakumar & Natarajan, 1989, 1990; Chinnakali, Selladurai, Sivakumar, Subramanian & Natarajan, 1990; Chinnakali, Sivakumar, Natarajan & Mathews, 1992).

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Structure of 3-*tert*-Butyl-1-[(4-chlorophenyl)sulfonyl]-1-methylurea

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Abstract. $C_{12}H_{17}ClN_2O_3S$, $M_r = 304.8$, triclinic, $P\bar{1}$, $a = 13.075(2)$, $b = 13.284(3)$, $c = 9.924(2)$ Å, $\alpha = 103.68(3)$, $\beta = 95.28(3)$, $\gamma = 66.34(4)°$, $V = 1534$ Å^3, $Z = 4$, $D_m = 1.33$, $D_x = 1.3197$ g cm^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1.54178$ Å, $\mu = 35.4$ cm^{-1}, $F(000) = 640$, $T = 296$ K, $R = 0.061$, $wR = 0.075$ for 4694 reflections [$I > 2\sigma(I)$]. There are two molecules in the asymmetric unit. In both molecules, the N atom attached to the *tert*-butyl group forms an intramolecular hydrogen bond with one of the sulfonyl O atoms, forming a six-membered ring. In the absence of intermolecular hydrogen bonds, the structure is stabilized by non-bonded interactions.

Experimental. Crystallization from petroleum ether, colourless thick-plate-shaped single crystal, 0.22 × 0.37 × 0.59 mm. The unit-cell parameters were refined from least-squares analysis of θ values for 29 reflections from $13.1 < \theta < 39.3°$. Intensities for 5822 unique reflections having $3 < \theta < 70°$, $-15 \le h \le 15$, $-16 \le k \le 15$, $0 \le l \le 12$, measured on a Siemens AED diffractometer, using ω–2θ scan mode, variable scan speed from 0.3 to 1.2° min^{-1}. During data collection, one standard reflection was monitored every 100 measurements with no decrease in intensity. The data were corrected for Lorentz and polarization effects. Absorption corrections were applied following Walker & Stuart (1983) after isotropic refinement using *ABSORB* (Ugozzoli, 1987). The

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