Related literature. Isolation from *Laurencia majuscula:* Caccamese & Compagnini (1989). Original determination, as ioslated from the sea hare, *Aplysia Californica,* which feeds on *Laurencia* species: Ireland, Stallard, Faulkner, Finer & Clardy (1976). Isolation from *Laurencia okamurai:* Oijka, Shizuri & Yamada (1982). Chemical constituents of *Laurencia* species: Erickson (1983), Faulkner (1984), Caccamese, Toscano, Cerrini & Gavuzzo (1982). Crystal structure of pacifenol, from *Laurencia majuscula:* Fronczek & Caccamese (1986). Crystal structure of dehydrochloroprepacifenol, from *Laurencia majuscula:* Caccamese, Compagnini, Toscano, Nicolo & Chapuis (1987). Criticism of original absolute configuration determination: Selover & Crews (1980).

References

CACCAMESE, S. & COMPAGNINI, A. (1989). *J. Nat. Prod.* Submitted.

CACCAMESE, S., COMPAGNINI, A., TOSCANO, R. M., NICOLO, F. & CHAPUIS, G. (1987). *Tetrahedron,* **43**, 5393–5399.

CACCAMESE, S., TOSCANO, R. M., CERRINI, S. & GAVUZZO, E. (1982). *Tetrahedron Lett.* pp. 3415–3418.

CROMER, D. T. (1974). *International Tables for X-ray Crystallography,* Vol. IV, Table 2.3.1. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography,* Vol. IV, Table 2.2B. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

ERICKSON, K. L. (1983). *Marine Natural Products,* Vol. 5, edited by P. J. SCHEUER, pp. 131–257. New York: Academic Press.

FAULKNER, D. J. (1984). *Nat. Prod. Rep.* **1**, 251–280.

FRENZ, B. A. & OKAYA, Y. (1980). *Enraf–Nonius Structure Determination Package.* Enraf–Nonius, Delft, The Netherlands.

FRONCZEK, F. R. & CACCAMESE, S. (1986). *Acta Cryst.* C**42**, 1649–1651.

HAMILTON, W. C. (1965). *Acta Cryst.* **18**, 502–510.

IRELAND, C., STALLARD, M. O., FAULKNER, D. J., FINER, J. & CLARDY, J. (1976). *J. Org. Chem.* **41**, 2461–2465.

OIJKA, M., SHIZURI, Y. & YAMADA, K. (1982). *Phytochemistry,* **21**, 2410–2411.

SELOVER, S. J. & CREWS, P. (1980). *J. Org. Chem.* **45**, 69–72.

Acta Cryst. (1989). C**45**, 1104–1105

Structure of 6-Benzyloxy-2,3-dichloro-4-(2-fluorobenzoyl)phenol

BY HIROSHI NAKAI

Shionogi Research Laboratories, Shionogi & Co. Ltd, Fukushima-ku, Osaka 553, Japan

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Abstract. $C_{20}H_{13}Cl_2FO_3$, $M_r = 391{\cdot}22$, monoclinic, $P2_1/c$, $a = 4{\cdot}932\ (1)$, $b = 20{\cdot}683\ (2)$, $c = 16{\cdot}831\ (2)$ Å, $\beta = 90{\cdot}14\ (1)°$, $V = 1717{\cdot}0\ (4)$ Å^3, $Z = 4$, $D_x = 1{\cdot}513$ Mg m^{-3}, $\lambda(\text{Cu } K\alpha) = 1{\cdot}54178$ Å, $\mu = 3{\cdot}66$ mm^{-1}, $F(000) = 800$, $T = 295$ K, $R = 0{\cdot}043$ for 2619 observed reflections [$F_o > 3\sigma(F_o)$]. The molecules are linked by an intermolecular hydrogen bond between O(24)H and O(8) to form an infinite chain extending along the c axis, O(24)H···O(8)(x, $\frac{3}{2}+y$, $\frac{1}{2}+z$) 1·96 (3) Å and O···O 2·792 (3) Å.

Experimental. Prismatic colorless crystals obtained from benzene. Crystal of dimensions 0·2 × 0·2 × 0·2 mm. Rigaku AFC-5 diffractometer, graphite-monochromatized Cu $K\alpha$. Cell dimensions determined from 2θ angles for 25 reflections in the range $30 < 2\theta < 50°$. Intensities measured up to $2\theta = 140°$ in h −5/0, k 0/25 and l −20/20, ω–2θ scans, ω-scan width $(1{\cdot}0 + 0{\cdot}2\tan\theta)°$, three standard reflections monitored every 100 measurements showed no significant change. 3193 unique reflections measured, 2619 intensities observed [$F_o \leq 3\sigma(F_o)$ and six very strong reflections rejected], no absorption corrections. Structure solved by *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). H atoms located on a difference density map. Positional and thermal parameters refined by block-diagonal least squares, isotropic for H and anisotropic for the others. $\sum(w|\Delta F|^2)$ minimized, $w = 1/[\sigma^2(F_o) + 0{\cdot}0008|F_o|^2]$, $w = 0$ for 64 reflections with $w^{1/2}|\Delta F| \geq 3$. Final $R = 0{\cdot}043$, $wR = 0{\cdot}049$, $S = 1{\cdot}1116$. Highest peak in final difference map 0·3 e Å^{-3}. Max. Δ/σ in the final cycle 0·03. Atomic scattering factors calculated by $\sum[a_i\exp(-b_i\lambda^{-2}\sin^2\theta)] + c$ $(i = 1,\ldots,4)$ (*International Tables for X-ray Crystallography,* 1974). Calculations performed on a FACOM M340R computer at Shionogi Research Laboratories. The final atomic coordinates and equivalent isotropic temperature factors are given in Table 1. Bond distances and angles are listed in Table 2.* A perspective view of the molecule with the

* Lists of structure factors, anisotropic temperature factors of the non-H atoms and atomic coordinates of the H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51727 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å²) *with e.s.d.'s in parentheses*

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

	x	y	z	B_{eq}
C(1)	−0·1346 (4)	0·7020 (1)	0·1877 (1)	3·14 (5)
C(2)	−0·1105 (5)	0·6731 (1)	0·2623 (1)	3·26 (5)
C(3)	−0·2654 (4)	0·6944 (1)	0·3259 (1)	3·12 (5)
C(4)	−0·4528 (4)	0·7441 (1)	0·3142 (1)	2·98 (5)
C(5)	−0·4727 (4)	0·7737 (1)	0·2412 (1)	2·97 (5)
C(6)	−0·3136 (4)	0·7532 (1)	0·1765 (1)	2·99 (5)
C(7)	−0·3537 (5)	0·7870 (1)	0·0997 (1)	3·34 (5)
O(8)	−0·3066 (4)	0·07612 (1)	0·0356 (1)	5·00 (5)
C(9)	−0·4682 (4)	0·8532 (1)	0·0987 (1)	3·24 (5)
C(10)	−0·3696 (5)	0·9034 (1)	0·1439 (1)	4·07 (6)
C(11)	−0·4710 (7)	0·9660 (1)	0·1383 (2)	5·86 (9)
C(12)	−0·6767 (7)	0·9777 (1)	0·0857 (2)	6·64 (10)
C(13)	−0·7780 (6)	0·9293 (2)	0·0393 (2)	6·31 (9)
C(14)	−0·6762 (5)	0·8678 (1)	0·0447 (1)	4·39 (7)
F(15)	−0·1630 (4)	0·8915 (1)	0·1945 (1)	5·98 (5)
O(16)	−0·6053 (3)	0·7576 (1)	0·3793 (1)	3·66 (4)
C(17)	−0·7785 (5)	0·8140 (1)	0·3787 (1)	3·82 (6)
C(18)	−0·6262 (4)	0·8761 (1)	0·3843 (1)	3·42 (5)
C(19)	−0·4180 (5)	0·8831 (1)	0·4398 (1)	4·10 (6)
C(20)	−0·2822 (6)	0·9410 (1)	0·4466 (2)	5·30 (8)
C(21)	−0·3503 (6)	0·9928 (1)	0·3998 (2)	5·42 (8)
C(22)	−0·5556 (6)	0·9870 (1)	0·3455 (2)	5·49 (8)
C(23)	−0·6931 (6)	0·9283 (1)	0·3367 (1)	4·66 (7)
O(24)	−0·2332 (4)	0·6663 (1)	0·3974 (1)	4·25 (4)
Cl(25)	0·1113 (1)	0·61019 (3)	0·27856 (4)	4·79 (2)
Cl(26)	0·0745 (1)	0·67453 (3)	0·11227 (3)	4·35 (2)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(1)–C(2)	1·395 (3)	C(9)–C(14)	1·402 (3)
C(1)–C(6)	1·391 (3)	C(10)–C(11)	1·391 (4)
C(1)–Cl(26)	1·733 (2)	C(10)–F(15)	1·349 (3)
C(2)–C(3)	1·388 (3)	C(11)–C(12)	1·366 (5)
C(2)–Cl(25)	1·721 (3)	C(12)–C(13)	1·364 (5)
C(3)–C(4)	1·396 (3)	C(13)–C(14)	1·370 (5)
C(3)–O(24)	1·345 (3)	O(16)–C(17)	1·446 (3)
C(4)–C(5)	1·376 (3)	C(17)–C(18)	1·491 (3)
C(4)–O(16)	1·359 (3)	C(18)–C(19)	1·394 (3)
C(5)–C(6)	1·409 (3)	C(18)–C(23)	1·384 (4)
C(6)–C(7)	1·482 (3)	C(19)–C(20)	1·377 (4)
C(7)–O(8)	1·226 (3)	C(20)–C(21)	1·371 (5)
C(7)–C(9)	1·481 (3)	C(21)–C(22)	1·368 (5)
C(9)–C(10)	1·375 (3)	C(22)–C(23)	1·398 (4)

C(2)–C(1)–C(6)	120·0 (2)	C(7)–C(9)–C(14)	119·0 (2)
C(2)–C(1)–Cl(26)	118·0 (2)	C(10)–C(9)–C(14)	117·0 (2)
C(6)–C(1)–Cl(26)	121·9 (2)	C(9)–C(10)–C(11)	122·6 (2)
C(1)–C(2)–C(3)	120·8 (2)	C(9)–C(10)–F(15)	118·5 (2)
C(1)–C(2)–Cl(25)	121·3 (2)	C(11)–C(10)–F(15)	118·9 (2)
C(3)–C(2)–Cl(25)	117·9 (2)	C(10)–C(11)–C(12)	118·4 (3)
C(2)–C(3)–C(4)	119·4 (2)	C(11)–C(12)–C(13)	120·8 (3)
C(2)–C(3)–O(24)	119·2 (2)	C(12)–C(13)–C(14)	120·6 (3)
C(4)–C(3)–O(24)	121·4 (2)	C(9)–C(14)–C(13)	120·7 (3)
C(3)–C(4)–C(5)	120·0 (2)	C(4)–O(16)–C(17)	119·2 (2)
C(3)–C(4)–O(16)	113·9 (2)	O(16)–C(17)–C(18)	113·4 (2)
C(5)–C(4)–O(16)	126·1 (2)	C(17)–C(18)–C(19)	120·1 (2)
C(4)–C(5)–C(6)	121·2 (2)	C(17)–C(18)–C(23)	121·1 (2)
C(1)–C(6)–C(5)	118·6 (2)	C(19)–C(18)–C(23)	118·8 (2)
C(1)–C(6)–C(7)	124·1 (2)	C(18)–C(19)–C(20)	120·2 (2)
C(5)–C(6)–C(7)	117·3 (2)	C(19)–C(20)–C(21)	120·9 (3)
C(6)–C(7)–O(8)	122·5 (2)	C(20)–C(21)–C(22)	119·7 (3)
C(6)–C(7)–C(9)	119·7 (2)	C(21)–C(22)–C(23)	120·3 (3)
O(8)–C(7)–C(9)	117·7 (2)	C(18)–C(23)–C(22)	120·1 (3)
C(7)–C(9)–C(10)	123·9 (2)		

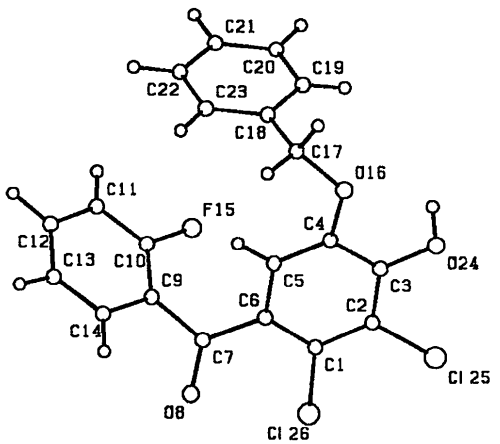

Fig. 1. Perspective view with the atom-numbering system.

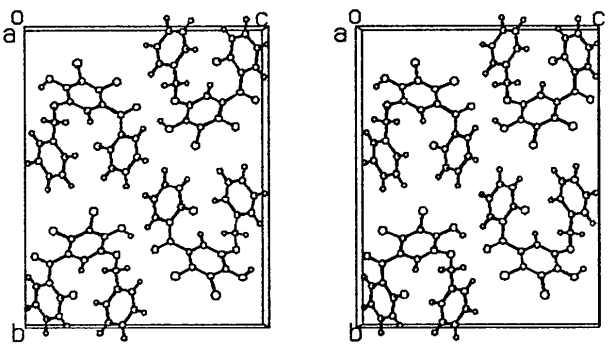

Fig. 2. A stereoview of the unit-cell packing.

atom-numbering system and a stereoview of the crystal packing drawn using the program *PLUTO* (Motherwell & Clegg, 1978) are presented in Figs. 1 and 2, respectively.

Related literature. The structure of the title compound has been discussed by Itazaki, Hayashi, Matsuura, Yonetani & Nakamura (1988).

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References

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

ITAZAKI, H., HAYASHI, K., MATSUURA, M., YONETANI, Y. & NAKAMURA, M. (1988). *Chem. Pharm. Bull.* **36**, 3404–3432.

MAIN, P., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO.* Program for plotting molecular and crystal structures. Univ. of Cambridge, England.