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Structure of the Methyl Ester of Everninic Acid (Methyl 2-Hydroxy-4-methoxy-6-methylbenzoate)

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Abstract. $C_{10}H_{12}O_4$, $M_r = 196.2$, monoclinic, $P2_1/n$, $a = 11.418$ (2), $b = 7.989$ (1), $c = 11.231$ (2) Å, $\beta = 106.36$ (1)°, $V = 983.0$ Å^3, $Z = 4$, D_m (flotation in KI/H_2O) = 1.30, $D_x = 1.326$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 0.10$ mm^{-1}, $F(000) = 416$, room temperature, $R = 0.045$, $wR = 0.078$ for 1107 observed reflections. The molecule is essentially planar with a strong intramolecular hydrogen bond involving the adjacent hydroxyl and carboxylate groups.

Experimental. The synthesis of the title compound (1) has been described previously (Nicollier, Rebetez, Tabacchi, Gerlach & Thalmann, 1978). Transparent block-like crystals of a synthetic sample of (1) were grown by slow evaporation of a concentrated solution in 1,2-dimethoxyethane. A crystal of dimensions 0.38 × 0.36 × 0.30 mm was used for data collection using a Stoe AED2 four-circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation. When mounted on a glass fiber the crystal melted in the X-ray beam (melting point 339–340 K). Hence the crystal was sealed in a Lindemann-glass capillary and suffered no thermal damage during data collection. < 2% intensity variation for 5 standard reflections measured every hour. Accurate cell parameters from $\pm\omega$ values of 25 reflections and their equivalents in the range $25 < 2\theta < 40°$. 3922 reflections were measured by the $\omega/2\theta$ scan mode with $\theta_{max} = 25°$, and index limits h −13 to 13, k −9 to 9, l 0 to 13. The systematic absences were consistent with space group $P2_1/n$. 1737 unique reflections, $R_{int} = 0.034$; 1107 [$I > 3.5\sigma(I)$] were considered observed and used for all further calculations. Structure solved using a combination of *SHELXS*86 (Sheldrick, 1986) and *PATSEE* (Egert, 1985). Refinement and all further calculations were carried out using the NRCVAX system (Gabe, Le Page, Charland & Lee, 1989). H atoms located from difference maps and refined isotropically. Weighted full-matrix least-squares refinement for 1107 reflections gave $R = 0.045$ and $wR = 0.078$; function minimized $\sum w(|F_o| - |F_c|)^2$, $w^{-1} = \sigma^2(F_o) + 0.002(F_o^2)$. In the final cycle of refinement the maximum shift/σ ratio was 0.022. Residual density limits in final difference map +0.16 and −0.20 e Å^{-3}. Neutral complex-atom scattering factors in *NRCVAX* from *International Tables for X-ray Crystallography* (1974, Vol. IV). Final positional† and equivalent isotropic thermal parameters are given in Table 1 and interatomic distances and angles in Table 2. The numbering scheme use is illustrated in Fig. 1.

Related literature. Simple monoaryl compounds are commonly found in mushrooms but are relatively rare in lichens (Culberson, 1969; Tabacchi &

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† Lists of structure factors, anisotropic thermal parameters, H-atom parameters, torsion angles and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54806 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AL0507]

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Table 1. *Atomic parameters x, y, z and B_{iso} values*

E.s.d.'s refer to the last digit printed.

	x	y	z	B_{iso}*(Å^2)
O(1)	0.8600 (2)	0.3695 (3)	0.9328 (2)	5.62 (12)
O(2)	0.9552 (2)	0.2186 (3)	0.8230 (2)	4.44 (9)
O(3)	0.7243 (2)	0.2332 (3)	1.0488 (2)	5.52 (11)
O(4)	0.6797 (2)	−0.3588 (3)	1.0253 (2)	5.18 (11)
C(1)	0.8264 (3)	0.0764 (3)	0.9218 (2)	3.66 (11)
C(2)	0.7510 (3)	0.0849 (4)	1.0023 (2)	3.90 (12)
C(3)	0.7008 (3)	−0.0559 (4)	1.0395 (2)	4.30 (13)
C(4)	0.7236 (3)	−0.2094 (4)	0.9956 (2)	3.84 (11)
C(5)	0.7948 (2)	−0.2237 (4)	0.9140 (2)	3.67 (11)
C(6)	0.8467 (2)	−0.0850 (3)	0.8764 (2)	3.28 (10)
C(7)	0.8808 (3)	0.2321 (3)	0.8940 (2)	3.96 (12)
C(8)	1.0075 (4)	0.3717 (5)	0.7925 (4)	5.49 (17)
C(9)	0.9214 (3)	−0.1145 (4)	0.7874 (3)	4.25 (14)
C(10)	0.6096 (4)	−0.3549 (7)	1.1121 (4)	6.34 (21)

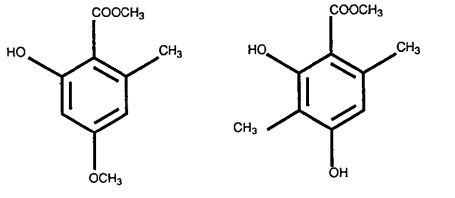
*B_{iso} is the mean of the principal axes of the thermal ellipsoids.

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

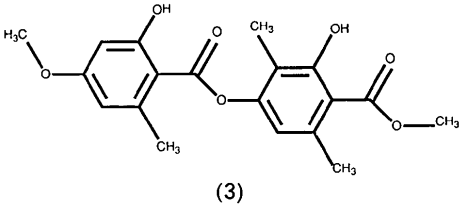
O(1)—C(7)	1.228 (4)	C(1)—C(6)	1.430 (4)
O(2)—C(7)	1.323 (4)	C(1)—C(7)	1.463 (4)
O(2)—C(8)	1.444 (4)	C(2)—C(3)	1.379 (4)
O(3)—C(2)	1.364 (3)	C(3)—C(4)	1.374 (4)
O(4)—C(4)	1.371 (3)	C(4)—C(5)	1.390 (4)
O(4)—C(10)	1.425 (4)	C(5)—C(6)	1.378 (4)
C(1)—C(2)	1.415 (4)	C(6)—C(9)	1.504 (4)
O(3)—H(O3)	1.05 (7)	O(1)···O(3)	2.534 (3)
		O(1)···H(O3)	1.55 (7)

C(7)—O(2)—C(8)	116.9 (3)	O(4)—C(4)—C(5)	114.3 (3)
C(4)—O(4)—C(10)	117.5 (3)	C(3)—C(4)—C(5)	121.0 (3)
C(2)—C(1)—C(6)	117.4 (2)	C(4)—C(5)—C(6)	121.2 (3)
C(2)—C(1)—C(7)	117.9 (2)	C(1)—C(6)—C(5)	119.3 (2)
C(6)—C(1)—C(7)	124.7 (3)	C(1)—C(6)—C(9)	123.9 (2)
O(3)—C(2)—C(1)	121.9 (3)	C(5)—C(6)—C(9)	116.8 (2)
O(3)—C(2)—C(3)	115.9 (2)	O(1)—C(7)—O(2)	120.5 (3)
C(1)—C(2)—C(3)	122.3 (3)	O(1)—C(7)—C(1)	123.2 (3)
C(2)—C(3)—C(4)	118.8 (3)	O(2)—C(7)—C(1)	116.3 (2)
O(4)—C(4)—C(3)	124.7 (3)	O(3)—H(O3)···O(1)	154 (5)

Nicollier, 1977; Nicollier *et al.*, 1978). Care must be taken when examining lichens, as these compounds can be the result of accidental decomposition of known constituents of lichens. In particular, evernic acid can be formed from the depside evernic acid or its methyl ester, evernin (3) (Nicollier *et al.*, 1978). The structures of natural samples of the second moiety of evernin, methyl β-orcinol carboxylate (2), and evernin (3) itself have been reported (Brehm, Stoeckli-Evans, Tabacchi & Bürgi, 1983; Stoeckli-Evans & Blaser, 1991; respectively). The relatively planar geometry of the molecule and the strong intramolecular hydrogen bonding observed in (1) are similar to that found in acetylcholine β-resorcylate (Jensen, 1975), 2,6-dihydroxy-3-methoxycarbonyl-4-methylbenzenesulfonate oxonium trihydrate (Hanson, 1987), and (2).



(1) (2)



(3)

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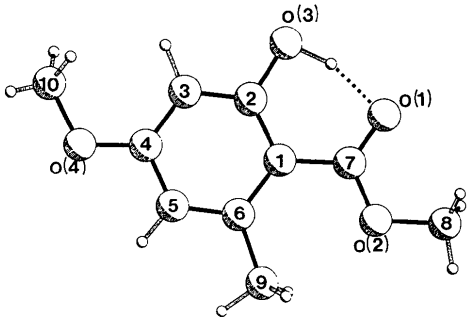

Fig. 1. *PLUTO* (Motherwell & Clegg, 1978) plot of (1) showing the numbering scheme.

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