

References

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Acta Cryst. (1995). **C51**, 709–712

Antifungal Compounds Isolated from New Zealand Flax: 7-Hydroxy-5-methoxy-6-methylphthalide and 4-Methoxycarbonyl- β -orcinol

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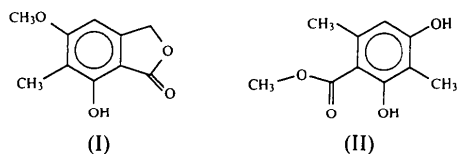
Abstract

7-Hydroxy-5-methoxy-6-methylphthalide, $C_{10}H_{10}O_4$, and the β -orcinol compound methyl 2,4-dihydroxy-3,6-dimethylbenzoate, $C_{10}H_{12}O_4$, were obtained from the hexane extracts of air-dried powdered roots of *Phormium cookianum* Le Jolis by column chromatography and repeated recrystallization from hexane/ether solution [Harvey & Waring (1987). *J. Nat. Prod.* **50**, 767–776]. X-ray analysis at low temperature (133 K) showed that crystals of the phthalide contain four independent hydrogen-bonded molecules, each of which has one intramolecular hydrogen bond. The five- and six-membered fused rings are planar with an average interplanar angle of 1.9° for three of the molecules, the rings being coplanar in the fourth, which has a weaker intramolecular hydrogen bond. The structure of methyl 2,4-dihydroxy-3,6-dimethylbenzoate at room temperature has been reported previously [Brehm, Stoeckli-Evans, Tabacchi & Bürgi (1983). *Helv. Chim. Acta*, **66**,

824–827]. The present low-temperature results are in close agreement with the previous results, the few minor differences being attributable to crystal-packing differences around the ester and hydroxyl groups.

Comment

The two extracts, 7-hydroxy-5-methoxy-6-methylphthalide, (I), and 4-methoxycarbonyl- β -orcinol, (II), from a flax plant, were obtained as part of a concerted study to identify the active ingredients used for curing various ills by New Zealand's Maori people. Neither could be identified uniquely by the usual spectroscopic methods [details of their antifungal properties are reported elsewhere (Harvey & Waring, 1987)].



The structure of (I) (Fig. 1) consists of four independent hydrogen-bonded molecules ($H \cdots O$ 2.02–2.29 Å; Table 3). Each of the molecules also has a longer intramolecular hydrogen bond ($H \cdots O$ 2.30–2.69 Å). Comparison of the four molecules confirms the definite planarity of the five- and six-membered rings; the interplanar angles are in the range 1.8 – 2.0° , except for that of molecule 2, which has a significantly weaker intramolecular hydrogen bond of distorted geometry resulting in the two fused rings being coplanar.

Small but significant deviations from the phthalide ring planes are observed for the carboxyl O [$O(n1)$] and methyl C atoms [$C(n10)$ and $C(n9)$, where n is the number of the molecule]. Ranges of equivalent bond

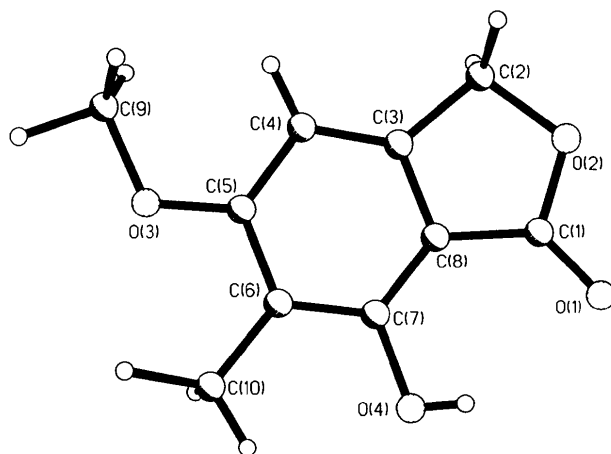


Fig. 1. View of the independent molecule in compound (I) (SHELXTL; Sheldrick, 1990). Atom labels in Tables 1 and 2 are based on those shown with a molecule number prefixed, e.g. C(21) is atom C(1) in molecule 2.

lengths and angles in the four molecules do not differ significantly except for those involving the methylene C atom of the five-membered ring. The average bond lengths and angles are not significantly different from those in the closely related compounds 4,7-dimethoxy-5-methylphthalide (Whalley, Ferguson & Roberts, 1980) and mycophenolic acid (Harrison, Shearer & Trotter, 1972). Similar geometry is also observed in relevant fragments of 8-acetyl-4,5-dihydro-1*H*,3*H*-naphtho[1,2-*c*:4,3-*b*]difuran-1-one (Watanabe, Kawada, Takamoto, Imada & Noguchi, 1984) and australide A (Horak, Steyn, Van Rooyen, Vlegaar & Rabie, 1981). The molecular packing is dominated by the hydrogen bonding between pairs of molecules (1 and 4, 2 and 3) with the mean planes of all molecules, except molecule 4, approximately normal to the *a* axis.

The structure of (II) (Fig. 2) has been described previously (Brehm, Stoekli-Evans, Tabacchi & Bürgi, 1983). Comparative statistics using χ^2 sums (Coppens *et al.*, 1987) and *t* tests indicate close agreement between the two studies (identical atom labels have been used). The volume decrease of the unit cell corresponding to the lower temperature of this study (27.3 Å³, 3%) is reflected in barely significant packing differences around the ester and hydroxyl groups [O(2) and O(10), respectively], and in a shortening of the intramolecular hydrogen-bond contact distance [H...O 1.66 (4) Å]. Final positional and equivalent isotropic displacement parameters are given in Table 4.

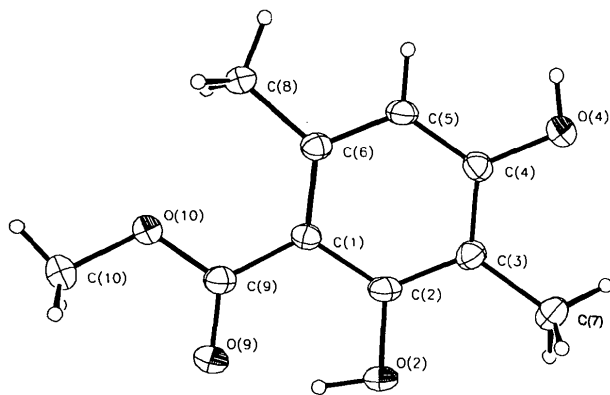


Fig. 2. View of compound (II) (ORTEP; Johnson, 1976) with 50% probability ellipsoids for non-H atoms.

Experimental

Compound (I)

Crystal data

C₁₀H₁₀O₄
M_r = 194.2

Mo K α radiation
 $\lambda = 0.71073$ Å

Triclinic
P $\bar{1}$
a = 6.985 (4) Å
b = 16.056 (22) Å
c = 16.566 (17) Å
 $\alpha = 81.92$ (10) $^\circ$
 $\beta = 85.05$ (7) $^\circ$
 $\gamma = 79.34$ (8) $^\circ$
V = 1804 (3) Å³
Z = 8
*D*_x = 1.43 Mg m⁻³

Data collection

Nicolet R3m diffractometer
 ω scans
Absorption correction:
none
4827 measured reflections
4665 independent reflections
1653 observed reflections
[*I* > 3 σ (*I*)]
*R*_{int} = 0.0195

Refinement

Refinement on *F*²
R(*F*) = 0.051
wR(*F*²) = 0.111
S = 1.110
4665 reflections
628 parameters
Only coordinates of H atoms
refined

Cell parameters from 24
reflections

$\theta = 3.5$ –13.7 $^\circ$
 $\mu = 0.12$ mm⁻¹
T = 133 K
Needle
0.50 × 0.12 × 0.08 mm
Light brown

$\theta_{\max} = 22.5^\circ$
h = 0 → 8
k = -18 → 18
l = -18 → 18
3 standard reflections
monitored every 97
reflections
intensity decay: 2%

$w = 1/[\sigma^2(F_o)^2 + 0.0702P^2]$
where $P = (F_o^2 + 2F_c^2)/3$
(Δ/σ)_{max} = 0.20
 $\Delta\rho_{\max} = 0.26$ e Å⁻³
 $\Delta\rho_{\min} = -0.26$ e Å⁻³
Atomic scattering factors
from *International Tables*
for *Crystallography* (1992,
Vol. C)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for (I)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
O(11)	0.2639 (11)	0.1136 (5)	0.4837 (5)	0.038 (2)
O(12)	0.2570 (10)	-0.0265 (5)	0.4972 (4)	0.031 (2)
O(13)	0.2723 (11)	-0.0630 (5)	0.8595 (4)	0.034 (2)
O(14)	0.2921 (12)	0.1669 (5)	0.6525 (4)	0.033 (2)
C(11)	0.2666 (17)	0.0464 (7)	0.5289 (7)	0.030 (3)
C(12)	0.2571 (19)	-0.0971 (8)	0.5645 (7)	0.030 (3)
C(13)	0.2660 (15)	-0.0578 (7)	0.6393 (7)	0.023 (3)
C(14)	0.2659 (17)	-0.0926 (7)	0.7206 (7)	0.028 (3)
C(15)	0.2687 (15)	-0.0362 (7)	0.7789 (7)	0.026 (3)
C(16)	0.2827 (16)	0.0514 (7)	0.7562 (8)	0.026 (3)
C(17)	0.2868 (15)	0.0809 (7)	0.6744 (7)	0.027 (3)
C(18)	0.2747 (15)	0.0284 (7)	0.6167 (6)	0.022 (3)
C(19)	0.2590 (24)	-0.1512 (8)	0.8871 (8)	0.052 (5)
C(110)	0.2868 (19)	0.1069 (8)	0.8206 (8)	0.034 (4)
O(21)	0.8158 (11)	-0.6848 (4)	0.9681 (5)	0.038 (2)
O(22)	0.7724 (11)	-0.6417 (4)	1.0925 (5)	0.037 (2)
O(23)	0.6960 (12)	-0.2744 (5)	0.9570 (5)	0.045 (2)
O(24)	0.7989 (14)	-0.5260 (5)	0.8384 (5)	0.044 (3)
C(21)	0.7870 (17)	-0.6263 (7)	1.0103 (8)	0.033 (3)
C(22)	0.7374 (20)	-0.5615 (8)	1.1256 (7)	0.033 (3)
C(23)	0.7367 (16)	-0.4936 (8)	1.0544 (7)	0.029 (3)
C(24)	0.7134 (18)	-0.4071 (8)	1.0490 (8)	0.038 (4)
C(25)	0.7180 (17)	-0.3610 (7)	0.9713 (8)	0.033 (3)
C(26)	0.7435 (16)	-0.3994 (7)	0.9016 (7)	0.028 (3)
C(27)	0.7720 (17)	-0.4888 (7)	0.9068 (7)	0.029 (3)
C(28)	0.7649 (15)	-0.5356 (7)	0.9857 (7)	0.025 (3)
C(29)	0.6786 (21)	-0.2295 (9)	1.0278 (10)	0.051 (4)
C(210)	0.7529 (21)	-0.3482 (9)	0.8177 (9)	0.043 (4)

O(31)	0.8650 (12)	0.3167 (5)	0.7807 (5)	0.042 (2)
O(32)	0.8289 (11)	0.2858 (4)	0.6547 (4)	0.032 (2)
O(33)	0.7670 (11)	-0.0749 (5)	0.7856 (4)	0.032 (2)
O(34)	0.8274 (12)	0.1633 (5)	0.9073 (5)	0.034 (2)
C(31)	0.8388 (16)	0.2665 (7)	0.7367 (7)	0.028 (3)
C(32)	0.8017 (18)	0.2092 (8)	0.6203 (7)	0.033 (3)
C(33)	0.7962 (15)	0.1405 (7)	0.6922 (7)	0.025 (3)
C(34)	0.7796 (15)	0.0567 (7)	0.6951 (7)	0.025 (3)
C(35)	0.7814 (16)	0.0097 (7)	0.7719 (7)	0.027 (3)
C(36)	0.7892 (16)	0.0457 (7)	0.8444 (7)	0.027 (3)
C(37)	0.8108 (16)	0.1285 (7)	0.8371 (7)	0.028 (3)
C(38)	0.8143 (16)	0.1783 (7)	0.7613 (7)	0.027 (3)
C(39)	0.7711 (20)	-0.1159 (8)	0.7143 (8)	0.034 (4)
C(310)	0.7836 (22)	-0.0076 (9)	0.9275 (8)	0.043 (4)
O(41)	0.3620 (10)	0.2834 (5)	0.5080 (4)	0.034 (2)
O(42)	0.3932 (10)	0.4219 (5)	0.4867 (4)	0.031 (2)
O(43)	-0.3180 (11)	0.5225 (4)	0.2968 (4)	0.031 (2)
O(44)	0.0124 (11)	0.2590 (4)	0.4192 (4)	0.030 (2)
C(41)	0.3015 (7)	0.3574 (8)	0.4771 (6)	0.030 (6)
C(42)	0.2875 (18)	0.5010 (7)	0.4433 (7)	0.029 (3)
C(43)	0.1230 (16)	0.4750 (6)	0.4092 (6)	0.020 (3)
C(44)	-0.0258 (18)	0.5231 (7)	0.3651 (7)	0.028 (3)
C(45)	-0.1625 (16)	0.4809 (7)	0.3404 (6)	0.023 (3)
C(46)	-0.1547 (16)	0.3916 (7)	0.3587 (6)	0.019 (3)
C(47)	0.0029 (17)	0.3459 (6)	0.4026 (6)	0.026 (3)
C(48)	0.1367 (16)	0.3879 (6)	0.4287 (6)	0.022 (3)
C(49)	-0.3461 (20)	0.6140 (8)	0.2800 (8)	0.038 (4)
C(410)	-0.3019 (19)	0.3466 (8)	0.3317 (8)	0.033 (3)

Compound (II)*Crystal data*C₁₀H₁₂O₄M_r = 196.2

Monoclinic

P2₁/c

a = 7.043 (2) Å

b = 18.142 (7) Å

c = 7.238 (2) Å

β = 96.44 (2)°

V = 918.9 (4) Å³

Z = 4

D_x = 1.42 Mg m⁻³*Data collection*

Nicolet R3m diffractometer

ω scans

Absorption correction:

none

2505 measured reflections

1415 observed reflections

[I > 3σ(I)]

R_{int} = 0.0134

Mo Kα radiation

λ = 0.71073 Å

Cell parameters from 24

reflections

θ = 3.7–16.5°

μ = 0.120 mm⁻¹

T = 133 K

Needle

0.38 × 0.23 × 0.13 mm

Light brown

θ_{max} = 27.5°

h = 0 → 10

k = 0 → 26

l = -11 → 11

3 standard reflections

monitored every 97

reflections

intensity decay: 2%

Refinement

Refinement on F

R = 0.040

wR = 0.052

S = 1.74

1415 reflections

175 parameters

All H-atom parameters

refined

w = 1/[σ²(F_o)
+ 0.0006(F_o)²](Δ/σ)_{max} = 0.004Δρ_{max} = 0.29 e Å⁻³Δρ_{min} = -0.21 e Å⁻³

Atomic scattering factors

from *International Tables*

for X-ray Crystallography

(1974, Vol. IV)

Table 4. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for (II)
$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U _{eq}
O(2)	1.3902 (2)	0.1890 (1)	0.2754 (2)	0.029 (1)
O(4)	0.7743 (2)	0.1122 (1)	0.0434 (2)	0.030 (1)
O(9)	1.4613 (2)	0.3265 (1)	0.3094 (2)	0.030 (1)
O(10)	1.2464 (2)	0.4092 (1)	0.1937 (2)	0.028 (1)
C(1)	1.1535 (3)	0.2839 (1)	0.1844 (2)	0.020 (2)
C(2)	1.2092 (3)	0.2087 (1)	0.2074 (2)	0.022 (2)
C(3)	1.0851 (3)	0.1504 (1)	0.1591 (3)	0.022 (2)
C(4)	0.8990 (3)	0.1684 (1)	0.0906 (2)	0.022 (2)
C(5)	0.8384 (3)	0.2416 (1)	0.0715 (3)	0.022 (2)
C(6)	0.9614 (3)	0.2996 (1)	0.1147 (2)	0.021 (2)
C(7)	1.1510 (4)	0.0720 (1)	0.1801 (3)	0.031 (2)
C(8)	0.8781 (3)	0.3760 (1)	0.0870 (3)	0.026 (2)
C(9)	1.2987 (3)	0.3398 (1)	0.2353 (3)	0.023 (2)
C(10)	1.3914 (3)	0.4651 (1)	0.2317 (4)	0.034 (2)

For compound (I), the H atoms were refined with three group isotropic U's for hydroxyl protons, methyl protons and ring protons.

Data collection, cell refinement and data reduction: *Nicolet R3m Software* (Siemens, 1983). Structure solution: *SHELXS86* (Sheldrick, 1985) and *MITHRIL* (Gilmore, 1984). Structure refinement: *SHELX76* (Sheldrick, 1976) and *SHELXL93* (Sheldrick, 1993). Molecular graphics: *ORTEPII* (Johnson, 1976) and *SHELXTL* (Sheldrick, 1990). Preparation of material for publication: *SHELX76* and *SHELXL93*.

Table 2. Selected geometric parameters (Å) for (I)

O(11)—C(11)	1.222 (12)	O(31)—C(31)	1.207 (12)
O(12)—C(11)	1.363 (12)	O(32)—C(31)	1.354 (12)
O(12)—C(12)	1.474 (12)	O(32)—C(32)	1.475 (14)
O(13)—C(15)	1.345 (12)	O(33)—C(35)	1.367 (12)
O(13)—C(19)	1.443 (14)	O(33)—C(39)	1.427 (14)
O(14)—C(17)	1.384 (13)	O(34)—C(37)	1.382 (13)
O(11)—C(18)	1.447 (14)	C(31)—C(38)	1.454 (14)
C(12)—C(13)	1.48 (2)	C(32)—C(33)	1.508 (14)
C(13)—C(14)	1.383 (14)	C(33)—C(34)	1.37 (2)
C(13)—C(18)	1.392 (14)	C(33)—C(38)	1.39 (2)
C(14)—C(15)	1.418 (14)	C(34)—C(35)	1.384 (14)
C(15)—C(16)	1.423 (14)	C(35)—C(36)	1.41 (2)
C(16)—C(17)	1.37 (2)	C(36)—C(37)	1.353 (14)
C(16)—C(110)	1.49 (2)	C(36)—C(310)	1.52 (2)
C(17)—C(18)	1.378 (14)	C(37)—C(38)	1.392 (14)
O(21)—C(21)	1.226 (12)	O(41)—C(41)	1.237 (12)
O(22)—C(21)	1.348 (13)	O(42)—C(41)	1.349 (12)
O(22)—C(22)	1.441 (12)	O(42)—C(42)	1.470 (12)
O(23)—C(25)	1.359 (12)	O(43)—C(45)	1.370 (12)
O(23)—C(29)	1.45 (2)	O(43)—C(49)	1.435 (13)
O(24)—C(27)	1.337 (13)	O(44)—C(47)	1.374 (11)
C(21)—C(28)	1.440 (14)	C(41)—C(48)	1.43 (2)
C(22)—C(23)	1.49 (2)	C(42)—C(43)	1.47 (2)
C(23)—C(24)	1.36 (2)	C(43)—C(44)	1.373 (14)
C(23)—C(28)	1.384 (14)	C(43)—C(48)	1.378 (14)
C(24)—C(25)	1.39 (2)	C(44)—C(45)	1.387 (14)
C(25)—C(26)	1.37 (2)	C(45)—C(46)	1.414 (13)
C(26)—C(27)	1.40 (2)	C(46)—C(47)	1.404 (14)
C(26)—C(210)	1.52 (2)	C(46)—C(410)	1.49 (2)
C(27)—C(28)	1.415 (14)	C(47)—C(48)	1.378 (14)

Table 3. Hydrogen-bonding geometry (Å, °) for (I)

D—H...A	H...A	D...A	D—H...A
O(14)—H(O14)...O(11)	2.41 (10)	3.07 (1)	144 (10)
O(24)—H(O24)...O(21)	2.69 (9)	3.09 (1)	118 (10)
O(34)—H(O34)...O(31)	2.41 (9)	3.04 (1)	133 (8)
O(44)—H(O44)...O(41)	2.30 (10)	3.07 (1)	136 (8)
O(14)—H(O14)...O(41)	2.29 (9)	2.88 (1)	136 (10)
O(24)—H(O24)...O(31 ⁱⁱ)	2.08 (10)	2.77 (1)	163 (11)
O(34)—H(O34)...O(21 ⁱⁱ)	2.11 (10)	2.75 (1)	134 (8)
O(44)—H(O44)...O(11)	2.02 (8)	2.79 (1)	135 (8)

Symmetry codes: (i) x, y - 1, z; (ii) x, 1 + y, z.

The author would like to thank H. E. Harvey and J. M. Waring for supplying the crystals.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates for (I) and (II), angles for (I) and bond lengths and angles for (II), have been deposited with the IUCr (Reference: AS1120). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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N-Hydroxyphthalimide

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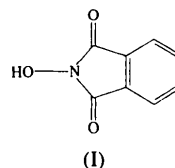
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Abstract

The title compound, *N*-hydroxy-1*H*-isoindole-1,3(2*H*)-dione, C₈H₅NO₃, is virtually planar with a maximum deviation of 0.03 (1) Å from planarity. Molecules are connected *via* hydrogen bonds and van der Waals interactions.

Comment

The title molecule, (I), is planar with a maximum deviation from the molecular plane of 0.03 (1) Å and a dihedral angle between the five- and six-membered ring planes of 0.66 (7)°. These features are similar to those found in ninhydrin (Medrud, 1969). Our interest is in comparing the geometries of the hydroxamic and amidic groups. Compared with the structure of phthalic anhydride (Bates & Cutler, 1977), the structure of the title compound shows only small differences in bond lengths between chemically equivalent atoms, but the N(1)—C(1)—O(1) [124.6 (5)°] and N(1)—C(2)—O(2) [124.9 (5)°] bond angles are about 4° larger than the corresponding angles of phthalic anhydride (120.5 and 120.6°, respectively) and are close to the corresponding angles in *N*-phthaloylglycine hydroxamic acid form (I) (123.5 and 124.0°, respectively) and form (II) (123.5 and 124.3°, respectively) (Sikirica & Vickovic, 1980, 1981).



The crystal structure is characterized by intermolecular hydrogen bonds: O(10)··O(1ⁱ) 2.69 (1) Å and O(10)—H(10)··O(1ⁱ) 167 (3)° [symmetry code: (i) 2−*x*, $\frac{1}{2}$ + *y*, $\frac{1}{2}$ − *z*]. These values are in good agreement with the values for salicylhydroxamic acid (Larsen, 1978), acetohydroxamic acid hemihydrate (Bracher & Small, 1970) and *N*-(3-cyanophenyl)acetohydroxamic acid hydrate (Mocharla, Powell & van der Helm, 1984).

The molecular packing is stabilized by hydrogen bonds and van der Waals interactions. In the *b* direction, the molecules are linked into chains by hydrogen bonds.

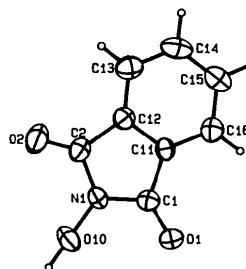


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are plotted at the 50% probability level.

Experimental

Crystal data

C₈H₅NO₃
M_r = 163.13

Mo *K*α radiation
 λ = 0.71073 Å