with the *A* ring system (C1–C5 and C10) to the extent that the sphere of influence of the methyl group (radius 2·28 Å) is only 0·08 Å from the van der Waals sphere of all H atoms bound to C2. This may be due to packing forces.

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Methyl 7-Methoxy-2-naphthoate

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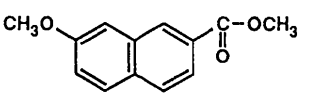
Abstract. $C_{13}H_{12}O_3$, $M_r = 216·2$, monoclinic, $P2_1/c$, $a = 3·9886$ (2), $b = 11·7995$ (9), $c = 22·789$ (3) Å, $\beta = 92·748$ (6)°, $V = 1071·3$ (3) Å^3, $Z = 4$, $D_x = 1·341$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 7·40$ cm^{-1}, $F(000) = 456$, $T = 295$ K, $R = 0·034$ for 1835 observations (of 2177 unique data). The average deviation from planarity is 0·007 Å with a maximum of 0·014 (1) Å for the fused rings. Both the methoxy and the carboxy groups are nearly coplanar with the naphthalene system. The CH_3O—C—C torsion angle is −1·5 (2)° with the methyl group *syn* to the neighboring α-carbon of the ring. In the ester the C—C—C—O torsion angles are −0·5 (2) with the methoxy O atom and 178·6 (1)° with the carbonyl O atom.

Experimental. The title compound (1), was prepared by the palladium-catalyzed reaction of carbon monoxide and methanol on the corresponding triflate



(1)

(Dolle, Schmidt & Kruse, 1987). Colorless laths of (1), m.p. 364·5–365·5 K, were isolated by recrystallization from ether. A fragment of size 0·15 × 0·35 × 0·38 mm, mounted on a glass fiber in random orientation, was used for data collection on an Enraf–Nonius CAD-4 diffractometer equipped with Cu $K\alpha$ radiation and a graphite monochromator. Cell dimensions from setting angles of 25 reflections having $25 < \theta < 30°$. Space group determined to be $P2_1/c$ from systematic absences $h0l$ with l odd, $0k0$ with k odd.

A hemisphere of data having $4 < 2\theta < 150°$, $0 \le h \le 4$, $-14 \le k \le 14$, $-28 \le l \le 28$ was collected using ω–2θ scans designed for $I = 25\sigma(I)$, subject to max. scan time = 60 s, scan rates varied 0·92–3·30° min^{-1}. Three reflections (100, 060, 008) were measured every 166 min, and their intensities exhibited only random fluctuations during data collection. A total of 4423 measurements was made. Lorentz and polarization corrections were applied. An empirical absorption correction based on a series of ψ scans was applied to the data. Relative transmission coefficients ranged from 0·8417 to 0·9962 with an average value of 0·9465. $R_{int} = 0·010$ for averaging the two equivalent quadrants. Structure solved by direct methods, using *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982), and refined by weighted full-matrix least squares; non-H atoms refined anisotropically; H atoms were located from difference maps and refined isotropically.

The function minimized was $\sum w(|F_o| - |F_c|)^2$ and weights were assigned as $w = 4F_o^2\mathrm{Lp}[S^2(C + R^2B) + (0·02F_o^2)^2]^{-1}$, where S = scan rate, C = total integrated peak count, R = scan time/background counting time, B = total background count, Lp = Lorentz–polarization factor, using Enraf–Nonius *SDP* (Frenz & Okaya, 1980), scattering factors of Cromer & Waber (1974), anomalous coefficients of Cromer (1974). Of 2177 unique data, 1835 reflections having $I > 3\sigma(I)$ were used in the refinement. The extinction coefficient (Larson, 1969) was refined in the least squares to $g = 1·54$ (8) × 10^{-5}, where the correction factor $(1 + gI_c)^{-1}$ was applied to F_c; maximum correction 53·1% for the $12\bar{2}$ reflection. The

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Table 1. *Coordinates and equivalent isotropic thermal parameters*

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

	x	y	z	B_{eq}(Å^2)
O1	0·9077 (2)	0·27510 (7)	0·97732 (3)	4·46 (2)
O2	0·6552 (3)	0·03412 (8)	0·62804 (4)	6·13 (2)
O3	0·4740 (2)	0·20112 (7)	0·65933 (3)	4·48 (2)
C1	0·9335 (3)	0·20401 (9)	0·93029 (4)	3·61 (2)
C2	1·1031 (3)	0·1013 (1)	0·94361 (5)	4·21 (2)
C3	1·1396 (3)	0·02214 (9)	0·90138 (5)	4·27 (2)
C4	1·0125 (3)	0·03970 (9)	0·84306 (5)	3·68 (2)
C5	1·0421 (3)	−0·04171 (9)	0·79798 (5)	4·39 (2)
C6	0·9171 (3)	−0·0213 (1)	0·74239 (5)	4·31 (2)
C7	0·7544 (3)	0·08261 (9)	0·72871 (4)	3·68 (2)
C8	0·7193 (3)	0·16288 (8)	0·77170 (4)	3·47 (2)
C9	0·8458 (3)	0·14379 (8)	0·82972 (4)	3·32 (2)
C10	0·8098 (3)	0·22582 (8)	0·87450 (4)	3·48 (2)
C11	0·6256 (3)	0·10072 (9)	0·66735 (5)	4·00 (2)
C12	0·7448 (3)	0·3810 (1)	0·96621 (5)	4·50 (2)
C13	0·3368 (4)	0·2243 (1)	0·60103 (5)	4·88 (3)

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

O1	C1	1·369 (1)		C4	C5	1·416 (2)	
O1	C12	1·425 (1)		C4	C9	1·423 (1)	
O2	C11	1·202 (1)		C5	C6	1·360 (2)	
O3	C11	1·339 (1)		C6	C7	1·415 (2)	
O3	C13	1·439 (1)		C7	C8	1·375 (1)	
C1	C2	1·414 (2)		C7	C11	1·482 (1)	
C1	C10	1·366 (1)		C8	C9	1·411 (1)	
C2	C3	1·354 (2)		C9	C10	1·419 (1)	
C3	C4	1·415 (2)					
C1	O1	C12	116·67 (8)	C6	C7	C8	120·1 (1)
C11	O3	C13	116·34 (9)	C6	C7	C11	117·87 (9)
O1	C1	C2	114·24 (9)	C8	C7	C11	122·05 (9)
O1	C1	C10	125·17 (9)	C7	C8	C9	120·93 (9)
C2	C1	C10	120·60 (9)	C4	C9	C8	118·73 (8)
C1	C2	C3	120·4 (1)	C4	C9	C10	119·85 (9)
C2	C3	C4	121·4 (1)	C8	C9	C10	121·42 (9)
C3	C4	C5	122·9 (1)	C1	C10	C9	119·77 (9)
C3	C4	C9	118·02 (9)	O2	C11	O3	122·5 (1)
C5	C4	C9	119·03 (9)	O2	C11	C7	124·6 (1)
C4	C5	C6	121·1 (1)	O3	C11	C7	112·97 (9)
C5	C6	C7	120·2 (1)				

final cycle included 194 variables and converged (largest $\Delta/\sigma = 0{\cdot}08$) with $R = 0{\cdot}034$, $wR = 0{\cdot}049$, R(all) = 0·039 and $S = 2{\cdot}691$. The max. residual density was 0·17, min. −0·12 e Å^{-3}. Table 1* presents the final coordinates and equivalent isotropic thermal parameters, Table 2 presents bond distances and angles. Fig. 1 illustrates the molecule and the numbering scheme, and Fig. 2 shows the unit cell.

Related literature. Crystal structures of several substituted 7-methoxy-2-naphthoates: Cameron, Feutrill, Pannan, Raston, Skelton & White (1981); Cameron, Feutrill, Lammerts van Bueren, Raston & White (1977); Akimoto & Iitaka (1969).

* Tables of H-atom coordinates, bond distances and angles involving H atoms, anisotropic thermal parameters, least-squares planes, and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54110 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

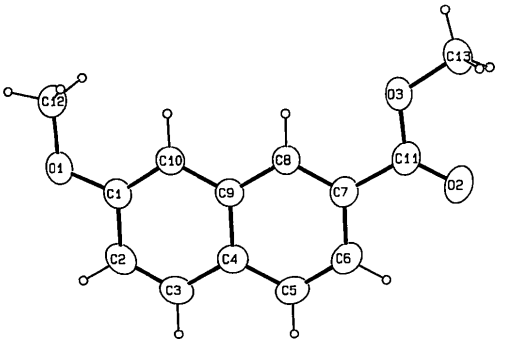

Fig. 1. Numbering scheme and thermal ellipsoids drawn at the 40% probability level. H atoms are drawn as circles with arbitrary radius.

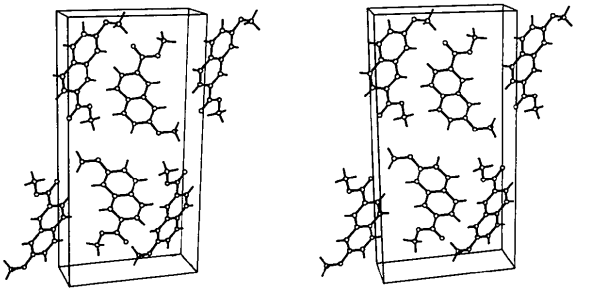

Fig. 2. Stereoview of the unit cell, viewed approximately down the *a* axis, with **b** horizontal.

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