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3-*endo*-(1-Naphthylamino)camphor

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Abstract. $C_{20}H_{23}NO$, $M_r = 293.41$, monoclinic, $C2/c$, $a = 25.515$ (3), $b = 7.0774$ (6), $c = 19.149$ (2) Å, $\beta = 108.12$ (1)°, $V = 3286.5$ (7) Å^3, $Z = 8$, $D_x = 1.190$ Mg m^{-3}, $\lambda(Cu\ K\alpha) = 1.54184$ Å, $\mu = 0.485$ mm^{-1}, $F(000) = 1264$, $T = 293$ K, final $R = 0.050$, $wR = 0.068$ for 2434 independent observed reflections. The geometry around the central N atom bridging the naphthyl and camphor moieties is: $N(1)–C(1') = 1.397$ (3), $N(1)–C(3) = 1.448$ (3) Å and $C(3)–N(1)–C(1') = 120.8$ (2)°. There are no unusually short contacts between the molecules.

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Experimental. The title compound was synthesized by the method of Forster and Spinner (Yagi, Ishige, Nagasawa & Maeda, 1989). Recrystallization from chloroform–ethanol (1:3 v/v) gave colorless needles; crystal size $0.4 \times 0.4 \times 0.2$ mm. Rigaku AFC-4 diffractometer, graphite-monochromated Cu $K\alpha$ radiation, ω–2θ scan technique; cell parameters refined by least squares on the basis of 15 independent 2θ values in the range of 43–59°; 2862 reflections measured,

Table 1. *Final atomic coordinates* ($\times 10^3$) *with their e.s.d.'s and equivalent isotropic thermal parameters* (Å^2) *for non-H atoms*

$$B_{eq} = \tfrac{4}{3}\Sigma_i \Sigma_j B_{ij} \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	B_{eq}
C(1)	8200 (1)	3834 (2)	1326 (1)	3.9
C(2)	8473 (1)	3124 (2)	783 (1)	3.7
C(3)	8889 (1)	1602 (2)	1169 (1)	3.7
C(4)	8844 (1)	1707 (3)	1951 (1)	4.2
C(5)	9097 (1)	3599 (3)	2283 (1)	5.4
C(6)	8672 (1)	5054 (3)	1848 (1)	5.4
C(7)	8218 (1)	2032 (3)	1797 (1)	4.4
C(8)	7850 (1)	449 (3)	1366 (2)	5.8
C(9)	8060 (1)	2388 (4)	2491 (1)	6.8
C(10)	7660 (1)	4851 (3)	984 (1)	5.2
C(1')	9818 (1)	614 (2)	1161 (1)	3.8
C(2')	9786 (1)	−1088 (3)	1497 (1)	4.7
C(3')	10191 (1)	−2470 (3)	1569 (1)	5.6
C(4')	10628 (1)	−2177 (3)	1326 (1)	5.3
C(5')	11145 (1)	−65 (3)	747 (1)	5.3
C(6')	11207 (1)	1638 (4)	452 (1)	5.7
C(7')	10814 (1)	3064 (3)	392 (1)	5.4
C(8')	10364 (1)	2749 (3)	615 (1)	4.3
C(9')	10284 (1)	999 (2)	920 (1)	3.7
C(10')	10688 (1)	−442 (3)	996 (1)	4.3
O(1)	8413 (1)	3718 (2)	172 (1)	5.3
N(1)	9417 (1)	2018 (2)	1067 (1)	4.5

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

|			
C(1)–C(2)	1.505 (2)	C(1)–C(6)	1.565 (3)
C(1)–C(7)	1.554 (3)	C(1)–C(10)	1.511 (3)
C(2)–C(3)	1.533 (2)	C(2)–O(1)	1.209 (2)
C(3)–C(4)	1.539 (3)	C(3)–N(1)	1.448 (3)
C(4)–C(5)	1.536 (3)	C(4)–C(7)	1.550 (3)
C(5)–C(6)	1.540 (3)	C(7)–C(8)	1.528 (3)
C(7)–C(9)	1.525 (4)	C(1')–C(2')	1.379 (3)
C(1')–C(9')	1.430 (2)	C(1')–N(1)	1.397 (3)
C(2')–C(3')	1.398 (3)	C(3')–C(4')	1.353 (3)
C(4')–C(10')	1.410 (3)	C(5')–C(6')	1.362 (4)
C(5')–C(10')	1.415 (3)	C(6')–C(7')	1.403 (4)
C(7')–C(8')	1.361 (3)	C(8')–C(9')	1.411 (3)
C(9')–C(10')	1.426 (2)		
C(2)–C(1)–C(6)	101.3 (1)	C(2)–C(1)–C(7)	101.0 (1)
C(2)–C(1)–C(10)	114.6 (2)	C(6)–C(1)–C(7)	101.8 (1)
C(6)–C(1)–C(10)	115.5 (2)	C(7)–C(1)–C(10)	120.0 (2)
C(1)–C(2)–C(3)	107.6 (1)	C(1)–C(2)–O(1)	127.3 (2)
C(3)–C(2)–O(1)	124.9 (2)	C(2)–C(3)–C(4)	100.6 (1)
C(2)–C(3)–N(1)	109.1 (1)	C(4)–C(3)–N(1)	118.4 (2)
C(3)–C(4)–C(5)	107.2 (2)	C(3)–C(4)–C(7)	101.9 (1)
C(5)–C(4)–C(7)	103.0 (2)	C(4)–C(5)–C(6)	103.0 (2)
C(1)–C(6)–C(5)	104.5 (2)	C(1)–C(7)–C(4)	94.3 (1)
C(1)–C(7)–C(8)	112.7 (2)	C(1)–C(7)–C(9)	113.7 (2)
C(4)–C(7)–C(8)	114.7 (2)	C(4)–C(7)–C(9)	113.2 (2)
C(8)–C(7)–C(9)	107.9 (2)	C(2')–C(1')–C(9')	119.5 (2)
C(2')–C(1')–N(1)	122.3 (2)	C(9')–C(1')–N(1)	118.2 (2)
C(1')–C(2')–C(3')	120.6 (2)	C(2')–C(3')–C(4')	121.5 (2)
C(3')–C(4')–C(10')	120.2 (2)	C(6')–C(5')–C(10')	121.4 (2)
C(5')–C(6')–C(7')	119.9 (2)	C(6')–C(7')–C(8')	120.5 (2)
C(7')–C(8')–C(9')	121.3 (2)	C(1')–C(9')–C(8')	122.9 (2)
C(1')–C(9')–C(10')	118.6 (2)	C(8')–C(9')–C(10')	118.4 (2)
C(4')–C(10')–C(5')	122.0 (2)	C(4')–C(10')–C(9')	119.5 (2)
C(5')–C(10')–C(9')	118.5 (2)	C(3)–N(1)–C(1')	120.8 (2)
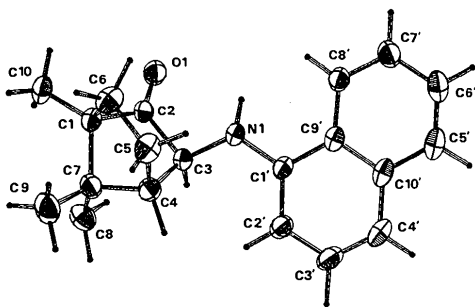
Fig. 1. ORTEP drawing (Johnson, 1965) of the title compound with atom numbering. The anisotropic ellipsoids for non-H atoms enclose 30% probability.
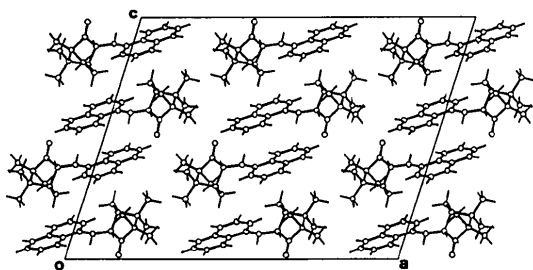
Fig. 2. A view of the unit cell.

using *SHELX*76 (Sheldrick, 1976), all H atoms are on the difference map; anisotropic temperature factors for all non-H atoms and isotropic temperature factors for H atoms using riding model with C—H 1·00 Å for the 9-methyl group; $R = 0.050$, $wR = 0.068$, $w^{-1} = \sigma^2(F) + 0.00625F^2$, $S = 1.06$, $(\Delta/\sigma)_{max} = 0.03$, largest peak in final ΔF map 0·12 e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1 contains final atomic coordinates and equivalent isotropic thermal parameters for non-H atoms.* Table 2 lists bond distances and angles. Fig. 1 shows the molecule and the numbering scheme adopted. Fig. 2 shows a view of the unit cell.

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* Lists of anisotropic thermal parameters for non-H atoms, positional and thermal parameters for H atoms, bond distances and angles, and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51769 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

2434 with $|F_o| > 3\sigma(|F_o|)$ used for structure determination, $2\theta_{max} = 125°$, *hkl* range: $h -29$ to 27, k 0–8, l 0–22, three standard reflections (02$\bar{9}$, 134 and 13,1,0) remeasured every 50 reflections without showing any significant change in intensity; corrections for Lorentz and polarization effects, absorption ignored; structure solved by direct methods with *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), refinement by full-matrix least squares on F

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Structure of Cinnamamide

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Abstract. C_9H_9NO, $M_r = 147.08$, m.p. $= 416$–418 K, monoclinic, $P2_1/a$, $a = 16.015$ (3), $b = 5.072$ (1), $c = 9.563$ (2) Å, $\beta = 93.99$ (2)°, $V = 775.0$ (3) Å^3, $Z = 4$, $D_m = 1.26$ (2), $D_x = 1.261$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1.5418$ Å, $\mu = 0.63$ mm^{-1}, $F(000) = 312$, $T = 295$ K, $R = 0.066$ for 1042 reflections with $|F_o| > 2\sigma(F_o)$. The C=C double bonds of the nearest neighbours are related by $\bar{1}$ with a C···C distance of 4·109 (4) Å, the interplanar spacing being 3·762 (4) Å for the planes through four C atoms involving the C=C bond. No topochemical reaction was observed.

Experimental. Crystals from a chloroform solution by slow evaporation. D_m by flotation in aqueous KI.

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