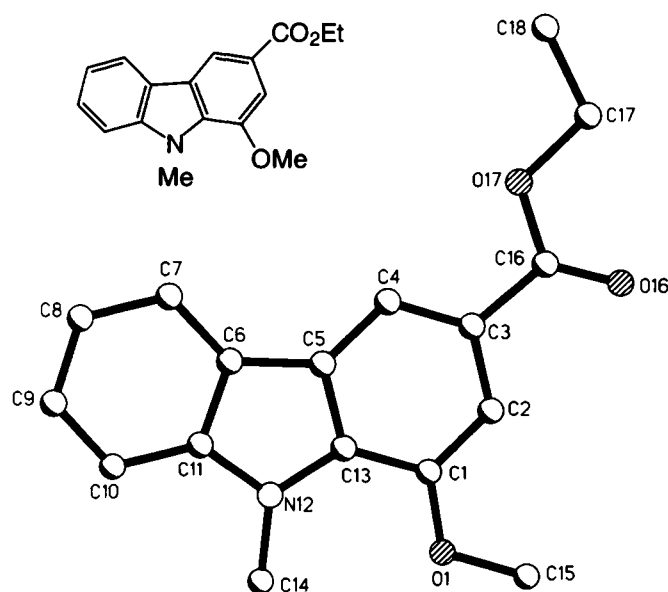


Crystal structure of ethyl 1-methoxy-9-methyl-9H-carbazol-3-carboxylate, $C_{12}NH_6(OCH_3)(CH_3)CO_2(C_2H_5)$

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**Table 1.** Data collection and handling.

Crystal:	colorless, lath, size 0.15 × 0.2 × 1.7 mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	0.89 cm ⁻¹
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{\max}$:	55°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	3488, 3346
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1914
$N(\text{param})_{\text{refined}}$:	190
Program:	SHELXTL-97 [2]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(2)	4e	0.1351	0.7698	1.0344	0.08
H(4)	4e	0.4222	0.4332	1.0835	0.08
H(7)	4e	0.6048	0.4673	1.1866	0.08
H(8)	4e	0.7254	0.5662	1.2802	0.08
H(9)	4e	0.6907	0.8894	1.3437	0.08
H(10)	4e	0.5350	1.1259	1.3158	0.08
H(14A)	4e	0.2622	1.2868	1.2137	0.08
H(14B)	4e	0.3760	1.3979	1.2421	0.08
H(14C)	4e	0.3296	1.1901	1.2789	0.08
H(15A)	4e	0.0187	1.2554	1.1034	0.08
H(15B)	4e	0.0216	0.9585	1.0850	0.08
H(15C)	4e	0.0606	1.1759	1.0471	0.08
H(17A)	4e	0.2619	0.1876	0.8938	0.08
H(17B)	4e	0.2330	-0.0347	0.9350	0.08
H(18A)	4e	0.3680	-0.1808	0.8951	0.08
H(18B)	4e	0.4095	-0.1627	0.9675	0.08
H(18C)	4e	0.4380	0.0579	0.9261	0.08

Abstract

$C_{17}H_{17}NO_3$, monoclinic, $P12_1/n1$ (No. 14), $a = 13.227(5)$ Å, $b = 5.083(1)$ Å, $c = 22.472(7)$ Å, $\beta = 106.16(3)^\circ$, $V = 1451.2$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.058$, $wR_{\text{ref}}(F^2) = 0.177$, $T = 293$ K.

Source of material

The title compound was prepared in 75 % yield by O- and N-deacetylation through solvolysis of ethyl 1-acetoxy-9-acetyl-9H-carbazole-3-carboxylate [1] with ethanol and K_2CO_3 followed by O- and N-methylation using dimethyl sulfate / K_2CO_3 in acetone.

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4e	0.2270(2)	0.9236(5)	1.1133(1)	0.058(1)	0.054(1)	0.050(1)	0.009(1)	0.023(1)	0.006(1)
O(1)	4e	0.1609(1)	1.1019(4)	1.12817(8)	0.063(1)	0.075(1)	0.064(1)	0.0204(9)	0.0205(8)	-0.0019(9)
C(2)	4e	0.2020(2)	0.7593(5)	1.0621(1)	0.055(1)	0.063(2)	0.050(1)	0.006(1)	0.014(1)	0.006(1)
C(3)	4e	0.2745(2)	0.5770(5)	1.0506(1)	0.057(1)	0.057(1)	0.041(1)	0.000(1)	0.014(1)	0.001(1)
C(4)	4e	0.3744(2)	0.5540(5)	1.09089(9)	0.056(1)	0.055(1)	0.044(1)	0.002(1)	0.018(1)	-0.001(1)
C(5)	4e	0.4017(2)	0.7175(5)	1.14315(9)	0.053(1)	0.050(1)	0.043(1)	0.001(1)	0.0191(9)	0.002(1)
C(6)	4e	0.4949(2)	0.7344(5)	1.19482(9)	0.054(1)	0.052(1)	0.042(1)	-0.003(1)	0.0185(9)	-0.000(1)
C(7)	4e	0.5901(2)	0.5970(5)	1.2122(1)	0.059(1)	0.061(2)	0.048(1)	0.002(1)	0.014(1)	-0.005(1)
C(8)	4e	0.6621(2)	0.6573(5)	1.2680(1)	0.060(1)	0.067(2)	0.056(1)	0.000(1)	0.009(1)	0.000(1)

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Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(9)	4e	0.6409(2)	0.8529(5)	1.3063(1)	0.071(2)	0.067(2)	0.048(1)	-0.009(1)	0.010(1)	-0.005(1)
C(10)	4e	0.5482(2)	0.9937(5)	1.2904(1)	0.072(2)	0.058(2)	0.050(1)	-0.008(1)	0.021(1)	-0.008(1)
C(11)	4e	0.4750(2)	0.9300(5)	1.2346(1)	0.059(1)	0.048(1)	0.045(1)	-0.004(1)	0.020(1)	-0.001(1)
N(12)	4e	0.3748(1)	1.0341(4)	1.20926(8)	0.062(1)	0.050(1)	0.049(1)	0.001(1)	0.0229(9)	-0.0047(9)
C(13)	4e	0.3292(2)	0.9029(4)	1.15409(9)	0.059(1)	0.050(1)	0.042(1)	-0.002(1)	0.022(1)	0.002(1)
C(14)	4e	0.3320(2)	1.2451(5)	1.2385(1)	0.075(2)	0.057(2)	0.071(2)	-0.001(1)	0.037(1)	-0.012(1)
C(15)	4e	0.0569(2)	1.1248(7)	1.0876(1)	0.064(2)	0.100(2)	0.083(2)	0.024(2)	0.022(2)	-0.007(2)
C(16)	4e	0.2395(2)	0.4111(5)	0.9943(1)	0.064(2)	0.061(2)	0.045(1)	0.004(1)	0.014(1)	0.002(1)
O(16)	4e	0.1510(1)	0.4098(4)	0.95959(8)	0.068(1)	0.101(2)	0.060(1)	0.014(1)	-0.0032(9)	-0.016(1)
O(17)	4e	0.3166(1)	0.2595(4)	0.98497(7)	0.065(1)	0.072(1)	0.0496(9)	0.0024(9)	0.0101(8)	-0.0173(9)
C(17)	4e	0.2878(2)	0.0859(6)	0.9315(1)	0.079(2)	0.072(2)	0.046(1)	0.006(2)	0.008(1)	-0.012(1)
C(18)	4e	0.3845(2)	-0.0633(7)	0.9299(1)	0.080(2)	0.094(2)	0.062(2)	-0.001(2)	0.021(1)	-0.024(2)

References

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