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Crystal structure of α-methyl-2-napthylmethanol, $C_{12}H_{11}OH$

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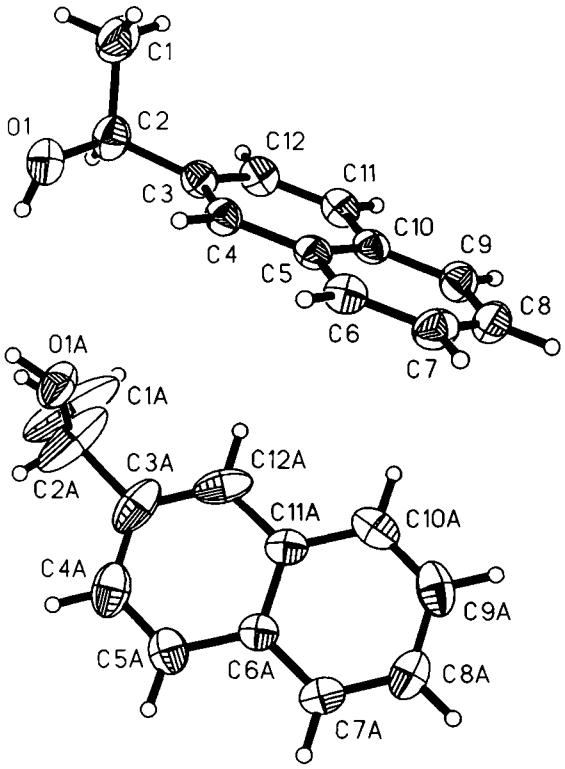

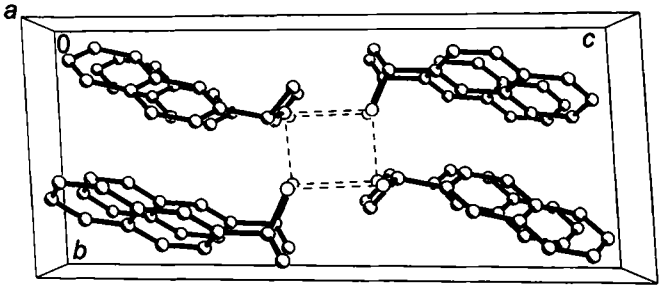

Abstract

$C_{12}H_{12}O$, triclinic, $P\bar{1}$ (no. 2), $a = 5.940(1)$ Å, $b = 8.187(2)$ Å, $c = 19.102(4)$ Å, $\alpha = 86.205(4)°$, $\beta = 84.394(4)°$, $\gamma = 88.966(4)°$, $V = 922.4$ Å^3, $Z = 4$, $R_{gt}(F) = 0.061$, $wR_{ref}(F^2) = 0.158$, $T = 193$ K.

Source of material

The title compound was purchased from Aldrich, and crystals were grown from a solution of dichloromethane which was layered with hexanes.

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Experimental details

One methyl-methanol moiety was found to be disordered and not resolved. A split into two sites creates better bond lengths, but improper bond angles, since the moiety bonds to an aromatic ring. OH/CH_3 disorder can be excluded due to the clear O–H···O bond.

Discussion

The title compound was structurally characterized in the course of studying crystallization properties of chiral compounds and their racemic mixtures. α-Methyl-2-napthylmethanol crystallizes with two molecules in the asymmetric unit (figure, top) and has a tetrameric nature when hydrogen bonding is included in the analysis (figure, bottom).

Table 1. Data collection and handling.

Crystal:	colorless needle, size 0.1 × 0.1 × 0.2 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.77 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5202, 3222
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2720
$N(param)_{refined}$:	239
Programs:	SHELXS-97 [1], SHELXL-97 [2], SHELXTL [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	2*i*	0.5921	0.4517	0.4170	0.071
H(1A)	2*i*	1.0148	0.3039	0.4932	0.084
H(1B)	2*i*	1.1988	0.2855	0.4271	0.084
H(1C)	2*i*	0.9933	0.1601	0.4415	0.084
H(2)	2*i*	0.9390	0.5014	0.4044	0.051
H(4)	2*i*	0.6532	0.2344	0.3107	0.038
H(6)	2*i*	0.5626	0.1049	0.2013	0.042
H(7)	2*i*	0.6628	0.0494	0.0853	0.048
H(8)	2*i*	1.0075	0.1420	0.0270	0.050
H(9)	2*i*	1.2543	0.2838	0.0854	0.045
H(11)	2*i*	1.3485	0.4078	0.1948	0.041
H(12)	2*i*	1.2516	0.4621	0.3104	0.043
H(1A1)	2*i*	0.3936	0.6555	0.4721	0.077
H(1A2)	2*i*	0.5935	0.9007	0.4678	0.223
H(1A3)	2*i*	0.6116	1.0070	0.3941	0.223
H(1A4)	2*i*	0.7666	0.8467	0.4037	0.223
H(2A)	2*i*	0.3217	0.8700	0.4116	0.118
H(4A)	2*i*	0.1251	0.9240	0.3210	0.062
H(5A)	2*i*	0.0631	0.9066	0.2060	0.050
H(7A)	2*i*	0.1827	0.8087	0.0868	0.047
H(8A)	2*i*	0.4428	0.6746	0.0128	0.056
H(9A)	2*i*	0.7801	0.5694	0.0541	0.061
H(10A)	2*i*	0.8530	0.5971	0.1684	0.053
H(12A)	2*i*	0.7242	0.6871	0.2897	0.060

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	2*i*	0.6640(3)	0.3641(2)	0.42473(9)	0.046(1)	0.056(1)	0.0386(9)	0.0038(8)	0.0043(8)	−0.0049(8)
C(1)	2*i*	1.0385(5)	0.2739(4)	0.4442(1)	0.051(2)	0.082(2)	0.037(1)	0.003(1)	−0.009(1)	−0.006(1)
C(2)	2*i*	0.8972(4)	0.3855(3)	0.3990(1)	0.044(1)	0.048(1)	0.036(1)	−0.004(1)	−0.002(1)	−0.009(1)
C(3)	2*i*	0.9412(4)	0.3509(3)	0.3220(1)	0.035(1)	0.030(1)	0.034(1)	0.0012(9)	−0.0028(9)	−0.0034(9)
C(4)	2*i*	0.7945(4)	0.2679(3)	0.2870(1)	0.028(1)	0.031(1)	0.034(1)	−0.0007(9)	0.0010(9)	0.0004(9)
C(5)	2*i*	0.8497(3)	0.2307(2)	0.2156(1)	0.030(1)	0.024(1)	0.034(1)	0.0016(8)	−0.0030(9)	0.0012(8)
C(6)	2*i*	0.7033(4)	0.1421(3)	0.1783(1)	0.034(1)	0.031(1)	0.040(1)	−0.0031(9)	−0.0052(9)	0.0003(9)
C(7)	2*i*	0.7623(4)	0.1094(3)	0.1096(1)	0.047(1)	0.037(1)	0.039(1)	−0.002(1)	−0.014(1)	−0.004(1)
C(8)	2*i*	0.9689(4)	0.1640(3)	0.0749(1)	0.053(2)	0.042(1)	0.030(1)	0.004(1)	−0.003(1)	−0.004(1)
C(9)	2*i*	1.1144(4)	0.2483(3)	0.1094(1)	0.039(1)	0.038(1)	0.035(1)	0.001(1)	0.003(1)	0.0007(9)
C(10)	2*i*	1.0601(4)	0.2837(2)	0.1805(1)	0 033(1)	0.024(1)	0.035(1)	0.0018(8)	−0.0016(9)	0.0012(8)
C(11)	2*i*	1.2076(4)	0.3711(3)	0.2178(1)	0.028(1)	0.031(1)	0.043(1)	−0.0037(9)	0.0009(9)	−0.0005(9)
C(12)	2*i*	1.1501(4)	0.4034(3)	0.2862(1)	0.032(1)	0.036(1)	0.042(1)	−0.0039(9)	−0.0054(9)	−0.006(1)
O(1A)	2*i*	0.4088(3)	0.6494(2)	0.42812(8)	0.073(1)	0.046(1)	0.0316(9)	−0.0035(9)	0.0061(9)	0.0047(7)
C(1A)	2*i*	0.618(1)	0.8960(6)	0.4164(2)	0.284(7)	0.106(3)	0.071(3)	−0.109(4)	−0.096(4)	0.038(2)
C(2A)	2*i*	0.4602(9)	0.8070(4)	0.3948(2)	0.192(5)	0.070(2)	0.036(2)	−0.066(3)	−0.028(2)	0.011(1)
C(3A)	2*i*	0.4291(6)	0.8037(3)	0.3172(1)	0.092(2)	0.043(1)	0.031(1)	−0.030(2)	−0.000(1)	0.001(1)
C(4A)	2*i*	0.2342(5)	0.8704(3)	0.2905(1)	0.063(2)	0.045(2)	0.045(2)	−0.015(1)	0.012(1)	−0.008(1)
C(5A)	2*i*	0.1976(4)	0.8603(3)	0.2224(1)	0.038(1)	0.037(1)	0.049(1)	−0.005(1)	0.005(1)	−0.004(1)
C(6A)	2*i*	0.3552(4)	0.7823(2)	0.1751(1)	0.032(1)	0.027(1)	0.036(1)	−0.0062(9)	−0.0029(9)	0.0030(9)
C(7A)	2*i*	0.3174(4)	0.7651(3)	0.1042(1)	0.040(1)	0.040(1)	0.039(1)	−0.006(1)	−0.010(1)	0.004(1)
C(8A)	2*i*	0.4713(5)	0.6867(3)	0.0602(1)	0.059(2)	0.048(1)	0.034(1)	−0.011(1)	0.002(1)	−0.005(1)
C(9A)	2*i*	0.6729(5)	0.6235(3)	0.0850(2)	0.049(2)	0.039(1)	0.060(2)	−0.004(1)	0.019(1)	−0.008(1)
C(10A)	2*i*	0.7153(4)	0.6392(3)	0.1526(1)	0.032(1)	0.033(1)	0.067(2)	−0.002(1)	−0.002(1)	0.004(1)
C(11A)	2*i*	0.5577(4)	0.7171(3)	0.1999(1)	0.034(1)	0.027(1)	0.041(1)	−0.0072(9)	−0.0058(9)	0.0060(9)
C(12A)	2*i*	0.5895(5)	0.7301(3)	0.2721(1)	0.060(2)	0.038(1)	0.054(2)	−0.018(1)	−0.029(1)	0.017(1)

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References

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