Crystal structure of (2*R*,3*S*)-3-*O*-benzyl-2-benzylamino-3,4-dihydroxybutane nitrile, C₁₈H₂₀N₂O₂

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Source of material: The title compound (see ref. 1) was prepared by addition of sodium cyanide to (-)-(2*R*)-*N*,*O*-dibenzylglyceraldehyde (see ref. 2).

In the crystal two intermolecular hydrogen bridges are found from NH/OH pairing of neighbouring molecules.

C₁₈H₂₀N₂O₂, orthorhombic, *P*2₁2₁2₁ (No. 19), *a* = 5.567(1) Å, *b* = 9.731(2) Å, *c* = 30.540(7) Å, *V* = 1654.4 Å³, *Z* = 4, *R*(*F*) = 0.075, *R*_w(*F*²) = 0.133.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless needle, size 0.05 x 0.2 x 0.7 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.78 cm ⁻¹
Diffractometer:	Nicolet P3
Scan mode:	Wyckoff
<i>T</i> _{measurement} :	293 K
$2\theta_{\max}$:	50°
<i>N</i> (<i>hkl</i>) _{unique} :	1439
Criterion for <i>I</i> _o :	<i>I</i> _o > 2 σ (<i>I</i> _o)
<i>N</i> (<i>param</i>) _{refined} :	200
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4 <i>a</i>	0.992(1)	0.3630(5)	-0.0283(2)	0.057
H(2)	4 <i>a</i>	1.034(1)	0.6051(6)	0.0107(2)	0.047
H(3)	4 <i>a</i>	1.140(1)	0.4140(6)	0.0526(2)	0.046
H(4A)	4 <i>a</i>	0.810(1)	0.2879(6)	0.0877(2)	0.059
H(4B)	4 <i>a</i>	0.648(1)	0.3413(6)	0.0491(2)	0.059
H(5)	4 <i>a</i>	0.8123(8)	0.1436(4)	0.0328(1)	0.082
H(7A)	4 <i>a</i>	1.164(2)	0.6677(9)	0.0853(3)	0.110
H(7B)	4 <i>a</i>	1.257(2)	0.5357(9)	0.1095(3)	0.110
H(9)	4 <i>a</i>	1.339(2)	0.7909(8)	0.1484(2)	0.085
H(10)	4 <i>a</i>	1.268(2)	0.894(1)	0.2143(3)	0.108
H(11)	4 <i>a</i>	0.933(2)	0.833(1)	0.2544(3)	0.125
H(12)	4 <i>a</i>	0.691(2)	0.657(1)	0.2299(3)	0.127
H(13)	4 <i>a</i>	0.767(2)	0.5552(9)	0.1639(2)	0.099
H(16A)	4 <i>a</i>	1.060(2)	0.6056(7)	-0.0676(2)	0.073
H(16B)	4 <i>a</i>	0.784(2)	0.5730(7)	-0.0702(2)	0.073
H(18)	4 <i>a</i>	0.687(2)	0.3324(8)	-0.1022(2)	0.083
H(19)	4 <i>a</i>	0.748(2)	0.193(1)	-0.1616(3)	0.103
H(20)	4 <i>a</i>	1.077(2)	0.221(1)	-0.2046(3)	0.110
H(21)	4 <i>a</i>	1.346(2)	0.395(1)	-0.1898(3)	0.099
H(22)	4 <i>a</i>	1.289(1)	0.5334(8)	-0.1292(2)	0.075

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
N(1)	4 <i>a</i>	0.961(1)	0.4496(5)	-0.0283(2)	0.060(4)	0.035(3)	0.048(3)	0.012(3)	0.008(3)	0.001(3)
C(2)	4 <i>a</i>	0.922(1)	0.5274(6)	0.0110(2)	0.027(4)	0.030(3)	0.060(4)	-0.006(3)	0.003(4)	-0.002(4)
C(3)	4 <i>a</i>	0.972(1)	0.4436(6)	0.0527(2)	0.035(4)	0.036(4)	0.045(4)	-0.003(4)	0.002(3)	-0.005(3)
C(4)	4 <i>a</i>	0.811(1)	0.3181(6)	0.0574(2)	0.050(4)	0.044(4)	0.054(4)	0.003(4)	0.001(4)	0.005(4)
O(5)	4 <i>a</i>	0.8988(8)	0.2113(4)	0.0303(1)	0.057(3)	0.042(3)	0.065(3)	-0.005(3)	0.010(3)	-0.001(2)
O(6)	4 <i>a</i>	0.9288(9)	0.5240(5)	0.0902(1)	0.050(3)	0.073(3)	0.059(3)	-0.002(3)	0.002(3)	-0.026(3)
C(7)	4 <i>a</i>	1.120(2)	0.5968(9)	0.1061(3)	0.097(8)	0.098(7)	0.079(6)	-0.038(7)	0.028(6)	-0.036(5)
C(8)	4 <i>a</i>	1.064(2)	0.6617(8)	0.1492(2)	0.074(6)	0.067(5)	0.051(5)	-0.015(6)	0.006(5)	-0.011(4)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(9)	4a	1.207(2)	0.7633(8)	0.1649(2)	0.090(7)	0.078(6)	0.045(5)	-0.012(6)	0.003(5)	0.001(4)
C(10)	4a	1.164(2)	0.826(1)	0.2041(3)	0.120(9)	0.087(7)	0.064(6)	-0.005(8)	-0.024(6)	-0.007(6)
C(11)	4a	0.967(2)	0.789(1)	0.2282(3)	0.13(1)	0.13(1)	0.050(5)	0.03(1)	-0.002(7)	-0.027(6)
C(12)	4a	0.822(2)	0.685(1)	0.2133(3)	0.095(8)	0.15(1)	0.071(7)	-0.005(9)	0.018(6)	-0.013(7)
C(13)	4a	0.869(2)	0.6239(9)	0.1741(2)	0.088(8)	0.098(7)	0.062(6)	-0.013(6)	0.012(5)	-0.011(5)
C(14)	4a	0.675(1)	0.5842(7)	0.0129(3)	0.047(4)	0.029(4)	0.052(4)	-0.002(4)	0.008(4)	0.000(3)
N(15)	4a	0.484(1)	0.6273(6)	0.0123(2)	0.046(4)	0.047(4)	0.112(5)	0.006(4)	0.006(5)	0.002(4)
C(16)	4a	0.943(2)	0.5319(7)	-0.0685(2)	0.073(6)	0.057(5)	0.053(4)	0.012(5)	0.007(5)	0.009(4)
C(17)	4a	0.985(1)	0.4467(8)	-0.1083(2)	0.043(5)	0.058(5)	0.041(4)	0.007(4)	0.007(4)	0.019(4)
C(18)	4a	0.823(2)	0.3449(8)	-0.1194(2)	0.043(5)	0.101(7)	0.064(5)	0.006(6)	0.002(5)	-0.001(5)
C(19)	4a	0.858(2)	0.262(1)	-0.1551(3)	0.083(8)	0.101(7)	0.074(6)	0.002(7)	-0.023(6)	-0.009(6)
C(20)	4a	1.052(2)	0.279(1)	-0.1807(3)	0.100(9)	0.114(9)	0.062(6)	0.031(8)	0.005(6)	-0.016(6)
C(21)	4a	1.214(2)	0.381(1)	-0.1717(3)	0.076(7)	0.107(7)	0.064(6)	0.025(6)	0.035(6)	0.031(6)
C(22)	4a	1.178(1)	0.4643(8)	-0.1353(2)	0.057(5)	0.064(5)	0.067(5)	0.006(5)	0.013(5)	0.016(5)

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