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rac-2-Methylamino-1,2-diphenylethanol

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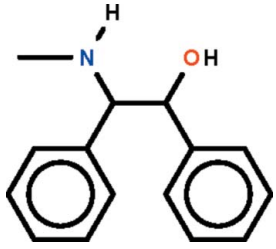
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.092; data-to-parameter ratio = 14.5.

The dihedral angle between the two phenyl rings in the title compound, $C_{15}H_{17}NO$, is 52.9 (1)°. In the crystal, the molecules are connected by O—H···N hydrogen bonds into centrosymmetric dimers. The amino H atom is not involved in hydrogen bonding.

Related literature

For the use of chiral 2-(2-methylamino)-1,2-diphenylethan-1-ol in organic synthesis, see: Gamsey *et al.* (2004).



Experimental

Crystal data

$C_{15}H_{17}NO$
M_r = 227.30
Monoclinic, $C2/c$
a = 27.4279 (7) Å
b = 5.69216 (11) Å
c = 17.1910 (5) Å
β = 116.223 (3)°
V = 2407.69 (10) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.838, T_{max} = 0.942
4176 measured reflections
2373 independent reflections
2197 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.03
2373 reflections
164 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1o···N1^{i}	0.92 (2)	1.88 (2)	2.799 (1)	172 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5789).

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supporting information

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rac-2-Methylamino-1,2-diphenylethanol

Ahmed Bari, Abdulrahman M. Al-Obaid and Seik Weng Ng

S1. Comment

Optically active 2-(2-methylamino)-1,2-diphenylethanol is used in asymmetric synthesis, *e.g.*, the asymmetric hydrogenation of chiral vinyloxazaboralidines (Gamsey *et al.*, 2004). The unsubstitued homolog is used for the palladium-assisted chiral tandem alkylation and carbonylative coupling reactions. The crystal structure of the *racemic* 2-(metahylamino)-1,2-diphenylethanol (Scheme I) is presented here.

The aromatic rings of the ethyl chain are staggered, the twist being 52.9 (1) °. The hydroxy group is hydrogen-bond donor to the amino group of an adjacent molecule; the amino group is hydrogen-bond donor to the hydroxy group of another molecule. The hydrogen bonds generate a linear chain running along [0 1 0] (Table 1).

S2. Experimental

The compound was obtained commercially, and crystals were grown from its solution in ethanol.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.95 to 1.0 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

The amino and hydroxy H-atoms were located in a difference Fourier map, and were freely refined.

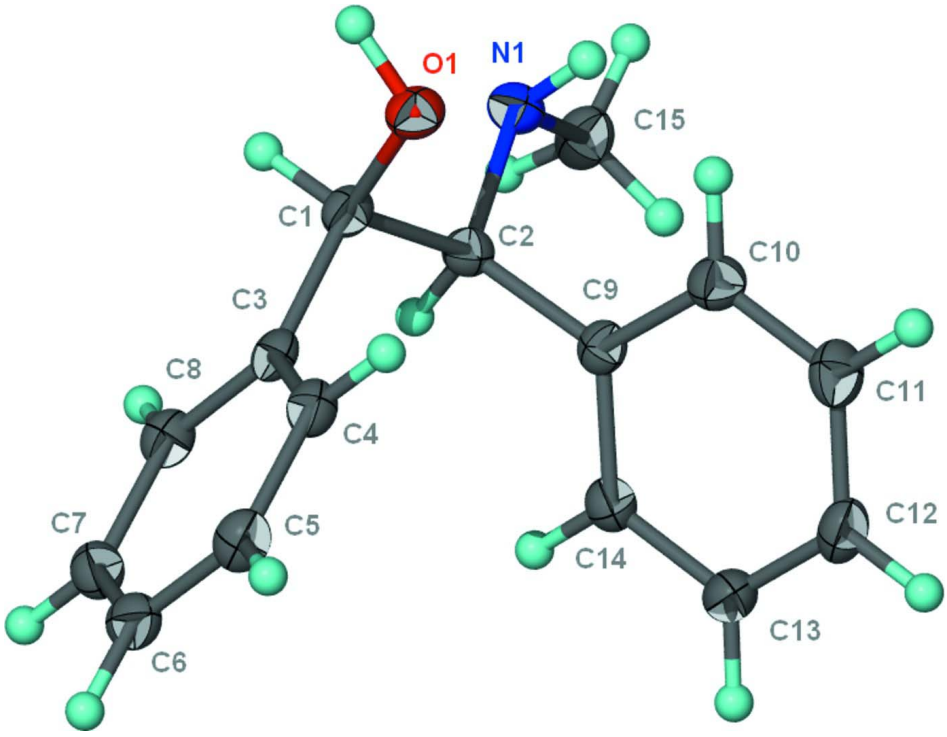

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{15}H_{17}NO$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

rac-2-Methylamino-1,2-diphenylethanol

Crystal data

$C_{15}H_{17}NO$
$M_r = 227.30$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 27.4279\ (7)$ Å
$b = 5.69216\ (11)$ Å
$c = 17.1910\ (5)$ Å
$\beta = 116.223\ (3)°$
$V = 2407.69\ (10)$ Å^3
$Z = 8$

$F(000) = 976$
$D_x = 1.254$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2861 reflections
$\theta = 2.9–74.3°$
$\mu = 0.61$ mm^{-1}
$T = 100$ K
Prism, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)

$T_{min} = 0.838$, $T_{max} = 0.942$
4176 measured reflections
2373 independent reflections
2197 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 74.5°$, $\theta_{min} = 3.6°$
$h = -26\rightarrow34$
$k = -6\rightarrow4$
$l = -19\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.092$
$S = 1.03$
2373 reflections
164 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 1.6566P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0042 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.56414 (3)	0.35675 (13)	0.57996 (5)	0.0187 (2)
N1	0.49951 (4)	0.73117 (17)	0.59666 (6)	0.0174 (2)
C1	0.57758 (4)	0.59658 (19)	0.57561 (7)	0.0159 (2)
H1	0.5564	0.6491	0.5142	0.019*
C2	0.55920 (4)	0.74825 (18)	0.63208 (7)	0.0152 (2)
H2	0.5679	0.9151	0.6250	0.018*
C3	0.63724 (4)	0.63255 (19)	0.59947 (6)	0.0157 (2)
C4	0.67644 (4)	0.46581 (19)	0.64578 (7)	0.0178 (2)
H4	0.6660	0.3244	0.6637	0.021*
C5	0.73091 (5)	0.5046 (2)	0.66609 (7)	0.0201 (3)
H5	0.7574	0.3897	0.6977	0.024*
C6	0.74656 (4)	0.7110 (2)	0.64018 (7)	0.0198 (3)
H6	0.7836	0.7365	0.6535	0.024*
C7	0.70781 (5)	0.8798 (2)	0.59482 (7)	0.0196 (3)
H7	0.7184	1.0217	0.5774	0.023*
C8	0.65356 (4)	0.84107 (19)	0.57486 (7)	0.0183 (2)
H8	0.6272	0.9575	0.5441	0.022*
C9	0.58952 (4)	0.69014 (19)	0.72835 (7)	0.0156 (2)
C10	0.57931 (5)	0.4847 (2)	0.76303 (7)	0.0203 (3)
H10	0.5521	0.3788	0.7263	0.024*
C11	0.60851 (5)	0.4332 (2)	0.85085 (7)	0.0220 (3)
H11	0.6011	0.2927	0.8735	0.026*
C12	0.64843 (5)	0.5860 (2)	0.90549 (7)	0.0215 (3)
H12	0.6685	0.5504	0.9654	0.026*
C13	0.65873 (4)	0.7908 (2)	0.87190 (7)	0.0217 (3)
H13	0.6859	0.8965	0.9089	0.026*
C14	0.62935 (4)	0.8422 (2)	0.78388 (7)	0.0184 (2)

H14	0.6367	0.9834	0.7615	0.022*
C15	0.47651 (5)	0.9274 (2)	0.62451 (7)	0.0219 (3)
H15A	0.4381	0.8962	0.6083	0.033*
H15B	0.4798	1.0722	0.5963	0.033*
H15C	0.4963	0.9453	0.6876	0.033*
H1O	0.5420 (7)	0.316 (3)	0.5233 (12)	0.047 (5)*
H1N	0.4909 (6)	0.597 (3)	0.6155 (9)	0.027 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0215 (4)	0.0148 (4)	0.0180 (4)	−0.0025 (3)	0.0070 (3)	−0.0017 (3)
N1	0.0150 (4)	0.0174 (5)	0.0190 (5)	−0.0005 (3)	0.0067 (4)	0.0003 (4)
C1	0.0181 (5)	0.0147 (5)	0.0137 (5)	−0.0001 (4)	0.0059 (4)	0.0001 (4)
C2	0.0149 (5)	0.0147 (5)	0.0153 (5)	−0.0006 (4)	0.0060 (4)	−0.0001 (4)
C3	0.0189 (5)	0.0170 (5)	0.0118 (5)	0.0000 (4)	0.0073 (4)	−0.0027 (4)
C4	0.0211 (5)	0.0176 (5)	0.0160 (5)	0.0003 (4)	0.0094 (4)	−0.0001 (4)
C5	0.0199 (5)	0.0219 (6)	0.0183 (5)	0.0044 (4)	0.0084 (4)	0.0010 (4)
C6	0.0185 (5)	0.0239 (6)	0.0184 (5)	−0.0002 (4)	0.0094 (4)	−0.0029 (4)
C7	0.0229 (6)	0.0186 (5)	0.0193 (5)	−0.0027 (4)	0.0112 (5)	−0.0013 (4)
C8	0.0207 (5)	0.0178 (5)	0.0161 (5)	0.0018 (4)	0.0077 (4)	0.0006 (4)
C9	0.0161 (5)	0.0168 (5)	0.0153 (5)	0.0020 (4)	0.0082 (4)	−0.0008 (4)
C10	0.0233 (6)	0.0179 (6)	0.0188 (5)	−0.0033 (4)	0.0085 (5)	−0.0019 (4)
C11	0.0283 (6)	0.0191 (6)	0.0210 (6)	0.0010 (5)	0.0131 (5)	0.0032 (4)
C12	0.0219 (5)	0.0283 (6)	0.0151 (5)	0.0034 (5)	0.0088 (4)	0.0025 (4)
C13	0.0192 (5)	0.0290 (6)	0.0164 (5)	−0.0050 (5)	0.0075 (5)	−0.0029 (5)
C14	0.0195 (5)	0.0193 (5)	0.0182 (5)	−0.0025 (4)	0.0098 (4)	−0.0004 (4)
C15	0.0203 (5)	0.0264 (6)	0.0196 (6)	0.0037 (4)	0.0093 (5)	−0.0008 (4)

Geometric parameters (Å, º)

O1—C1	1.4246 (13)	C7—C8	1.3888 (15)
O1—H1o	0.922 (18)	C7—H7	0.9500
N1—C15	1.4636 (14)	C8—H8	0.9500
N1—C2	1.4764 (13)	C9—C14	1.3900 (15)
N1—H1n	0.899 (15)	C9—C10	1.3961 (15)
C1—C3	1.5147 (14)	C10—C11	1.3922 (16)
C1—C2	1.5409 (14)	C10—H10	0.9500
C1—H1	1.0000	C11—C12	1.3889 (17)
C2—C9	1.5242 (14)	C11—H11	0.9500
C2—H2	1.0000	C12—C13	1.3842 (16)
C3—C4	1.3907 (15)	C12—H12	0.9500
C3—C8	1.3985 (15)	C13—C14	1.3953 (15)
C4—C5	1.3934 (15)	C13—H13	0.9500
C4—H4	0.9500	C14—H14	0.9500
C5—C6	1.3900 (16)	C15—H15A	0.9800
C5—H5	0.9500	C15—H15B	0.9800
C6—C7	1.3887 (16)	C15—H15C	0.9800

C6—H6	0.9500

C1—O1—H1O	104.6 (11)	C6—C7—H7	120.0
C15—N1—C2	111.99 (9)	C8—C7—H7	120.0
C15—N1—H1N	107.9 (9)	C7—C8—C3	120.75 (10)
C2—N1—H1N	109.2 (9)	C7—C8—H8	119.6
O1—C1—C3	112.89 (8)	C3—C8—H8	119.6
O1—C1—C2	109.85 (8)	C14—C9—C10	118.25 (10)
C3—C1—C2	111.63 (8)	C14—C9—C2	119.79 (9)
O1—C1—H1	107.4	C10—C9—C2	121.95 (10)
C3—C1—H1	107.4	C11—C10—C9	120.78 (10)
C2—C1—H1	107.4	C11—C10—H10	119.6
N1—C2—C9	114.03 (8)	C9—C10—H10	119.6
N1—C2—C1	108.37 (8)	C12—C11—C10	120.36 (11)
C9—C2—C1	112.89 (8)	C12—C11—H11	119.8
N1—C2—H2	107.1	C10—C11—H11	119.8
C9—C2—H2	107.1	C13—C12—C11	119.37 (10)
C1—C2—H2	107.1	C13—C12—H12	120.3
C4—C3—C8	118.85 (10)	C11—C12—H12	120.3
C4—C3—C1	122.15 (10)	C12—C13—C14	120.16 (11)
C8—C3—C1	119.00 (9)	C12—C13—H13	119.9
C3—C4—C5	120.48 (10)	C14—C13—H13	119.9
C3—C4—H4	119.8	C13—C14—C9	121.09 (10)
C5—C4—H4	119.8	C13—C14—H14	119.5
C6—C5—C4	120.17 (10)	C9—C14—H14	119.5
C6—C5—H5	119.9	N1—C15—H15A	109.5
C4—C5—H5	119.9	N1—C15—H15B	109.5
C7—C6—C5	119.77 (10)	H15A—C15—H15B	109.5
C7—C6—H6	120.1	N1—C15—H15C	109.5
C5—C6—H6	120.1	H15A—C15—H15C	109.5
C6—C7—C8	119.97 (10)	H15B—C15—H15C	109.5

C15—N1—C2—C9	73.91 (11)	C6—C7—C8—C3	−0.40 (16)
C15—N1—C2—C1	−159.45 (9)	C4—C3—C8—C7	1.16 (15)
O1—C1—C2—N1	−62.37 (10)	C1—C3—C8—C7	−179.41 (9)
C3—C1—C2—N1	171.61 (8)	N1—C2—C9—C14	−130.40 (10)
O1—C1—C2—C9	64.92 (11)	C1—C2—C9—C14	105.35 (11)
C3—C1—C2—C9	−61.09 (11)	N1—C2—C9—C10	50.82 (13)
O1—C1—C3—C4	−18.78 (14)	C1—C2—C9—C10	−73.43 (12)
C2—C1—C3—C4	105.54 (11)	C14—C9—C10—C11	−0.34 (16)
O1—C1—C3—C8	161.81 (9)	C2—C9—C10—C11	178.45 (10)
C2—C1—C3—C8	−73.87 (12)	C9—C10—C11—C12	−0.04 (17)
C8—C3—C4—C5	−0.97 (15)	C10—C11—C12—C13	0.32 (17)
C1—C3—C4—C5	179.62 (10)	C11—C12—C13—C14	−0.23 (17)
C3—C4—C5—C6	0.04 (16)	C12—C13—C14—C9	−0.16 (17)
C4—C5—C6—C7	0.74 (16)	C10—C9—C14—C13	0.44 (16)
C5—C6—C7—C8	−0.55 (16)	C2—C9—C14—C13	−178.38 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1o···N1^{i}	0.92 (2)	1.88 (2)	2.799 (1)	172 (2)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.