Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

rac-2-Amino-1,2-diphenylethanol

Ahmed Bari,[a] Abdulrahman M. Al-Obaid[a] and Seik Weng Ng[b,c]*

[a]Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

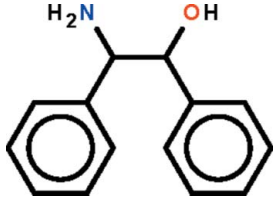
Received 15 January 2012; accepted 16 January 2012

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.085; data-to-parameter ratio = 14.3.

In the title compound, $C_{14}H_{15}NO$, the torsion angle about the two Csp^3 atoms adopts a partially eclipsed conformation [−61.5 (1)°]. The dihedral angle between the two rings is 48.1 (1)°. In the crystal, the molecules are connected by O—H···N and N—H···O hydrogen bonds into zigzag chains running along [010]. One of the amino H atoms is not involved in hydrogen bonding.

Related literature

For the use of chiral 2-amino-1,2-diphenylethan-1-ol in organic synthesis, see: Masters & Hegedus (1993); Masters *et al.* (1991).



Experimental

Crystal data

$C_{14}H_{15}NO$
M_r = 213.27
Monoclinic, $C2/c$
a = 26.6096 (6) Å
b = 5.3869 (1) Å
c = 17.1043 (4) Å
β = 114.689 (3)°
V = 2227.66 (8) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.63 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.859, T_{max} = 0.912
7706 measured reflections
2252 independent reflections
2139 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.00
2252 reflections
158 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.93 (2)	1.89 (2)	2.813 (1)	172 (2)
N1—H11···O1^{ii}	0.91 (2)	2.38 (2)	3.178 (1)	148 (1)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+2, -z+1$.

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).

We thank the Research Center of Pharmacy, King Saud University, and the Ministry of Higher Education of Malaysia (grant No. UM·C/HIR/MOHE/SC/12) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5788).

References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Masters, J. J. & Hegedus, L. S. (1993). *J. Org. Chem.* **58**, 4547–4554.
Masters, J. J., Hegedus, L. S. & Tamariz, J. (1991). *J. Org. Chem.* **56**, 5666–5671.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2012). E**68**, o491 [doi:10.1107/S1600536812002000]

rac-2-Amino-1,2-diphenylethanol

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

S1. Comment

Optically active 2-amino-1,2-diphenylethanol is commonly used for palladium-assisted chiral tandem alkylation and carbonylative coupling reactions (Masters & Hegedus, 1993; Masters *et al.*, 1991). The crystal structure of either one of the chiral enantiomers has not been reported although the crystal structures of several 2-ammonium-1,2-diphenylethanol carboxylates have been reported. The crystal structure of the racemic 2-amino-1,2-diphenylethanol (Scheme I) is presented here.

The aromatic rings of the ethyl chain of staggered, the twist being 48.1 (1) ° (Fig. 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). The amino group uses only one H atom to form a hydrogen bond.

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.

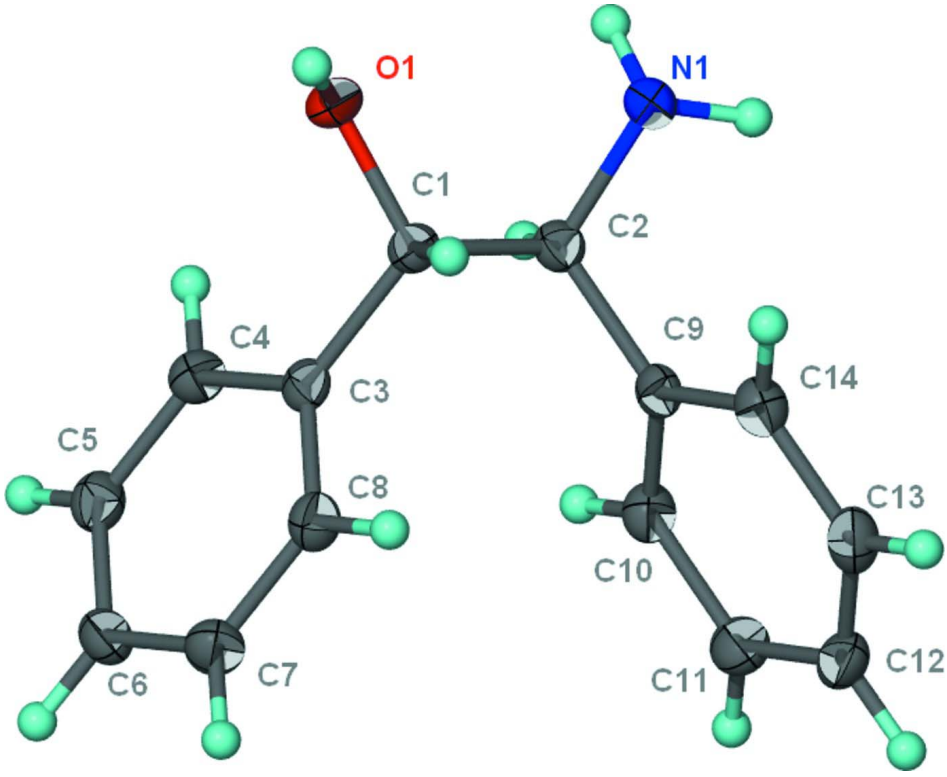


Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{14}H_{15}NO$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

rac-2-Amino-1,2-diphenylethanol

Crystal data

$C_{14}H_{15}NO$
$M_r = 213.27$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 26.6096$ (6) Å
$b = 5.3869$ (1) Å
$c = 17.1043$ (4) Å
$\beta = 114.689$ (3)°
$V = 2227.66$ (8) Å^3
$Z = 8$
$F(000) = 912$
$D_x = 1.272$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 5244 reflections
$\theta = 2.8$–$74.2°$
$\mu = 0.63$ mm^{-1}
$T = 100$ K
Prism, colorless
0.25 × 0.20 × 0.15 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)
$T_{min} = 0.859$, $T_{max} = 0.912$
7706 measured reflections
2252 independent reflections
2139 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 74.4°$, $\theta_{min} = 3.7°$
$h = -27\rightarrow32$
$k = -5\rightarrow6$
$l = -21\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.085$
$S = 1.00$
2252 reflections
158 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
$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 1.7088P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0028 (2)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.54033 (3)	0.71776 (14)	0.48409 (4)	0.01865 (19)
N1	0.49273 (3)	0.74451 (17)	0.59788 (6)	0.0188 (2)
C1	0.57362 (4)	0.64493 (18)	0.57066 (6)	0.0155 (2)
H1A	0.5680	0.4635	0.5765	0.019*
C2	0.55297 (4)	0.78952 (18)	0.62945 (6)	0.0158 (2)
H2	0.5593	0.9708	0.6247	0.019*
C3	0.63447 (4)	0.68973 (18)	0.59384 (6)	0.0153 (2)
C4	0.65167 (4)	0.89815 (19)	0.56318 (6)	0.0178 (2)
H4	0.6251	1.0145	0.5278	0.021*
C5	0.70746 (4)	0.93689 (19)	0.58397 (6)	0.0192 (2)
H5	0.7188	1.0799	0.5630	0.023*
C6	0.74672 (4)	0.7676 (2)	0.63521 (6)	0.0195 (2)
H6	0.7848	0.7934	0.6487	0.023*
C7	0.73012 (4)	0.56042 (19)	0.66658 (6)	0.0205 (2)
H7	0.7568	0.4444	0.7020	0.025*
C8	0.67424 (4)	0.52294 (19)	0.64605 (6)	0.0179 (2)
H8	0.6631	0.3815	0.6680	0.021*
C9	0.58301 (4)	0.71185 (18)	0.72263 (6)	0.0155 (2)
C10	0.62569 (4)	0.85732 (19)	0.77983 (6)	0.0187 (2)
H10	0.6360	1.0050	0.7599	0.022*
C11	0.65356 (4)	0.7899 (2)	0.86577 (6)	0.0222 (2)
H11A	0.6827	0.8911	0.9040	0.027*
C12	0.63889 (4)	0.5752 (2)	0.89591 (6)	0.0215 (2)
H12A	0.6576	0.5300	0.9548	0.026*
C13	0.59667 (4)	0.42707 (19)	0.83945 (7)	0.0208 (2)
H13	0.5866	0.2794	0.8597	0.025*
C14	0.56900 (4)	0.49391 (19)	0.75318 (6)	0.0187 (2)
H14	0.5404	0.3905	0.7148	0.022*
H1	0.5299 (6)	0.572 (3)	0.4526 (11)	0.044 (4)*
H11	0.4750 (6)	0.857 (3)	0.5560 (9)	0.029 (3)*
H12	0.4821 (6)	0.777 (3)	0.6421 (9)	0.029 (3)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0175 (3)	0.0230 (4)	0.0130 (3)	−0.0004 (3)	0.0041 (3)	0.0008 (3)
N1	0.0144 (4)	0.0250 (5)	0.0170 (4)	0.0014 (3)	0.0066 (3)	0.0016 (3)
C1	0.0156 (4)	0.0167 (5)	0.0133 (4)	−0.0006 (4)	0.0052 (4)	0.0004 (3)
C2	0.0149 (5)	0.0162 (5)	0.0165 (5)	−0.0004 (3)	0.0067 (4)	0.0005 (3)
C3	0.0169 (5)	0.0171 (5)	0.0126 (4)	−0.0008 (4)	0.0069 (4)	−0.0029 (3)
C4	0.0183 (5)	0.0176 (5)	0.0166 (4)	0.0008 (4)	0.0064 (4)	0.0010 (4)
C5	0.0212 (5)	0.0192 (5)	0.0183 (5)	−0.0036 (4)	0.0094 (4)	−0.0003 (4)
C6	0.0156 (5)	0.0241 (5)	0.0196 (5)	−0.0015 (4)	0.0082 (4)	−0.0021 (4)
C7	0.0186 (5)	0.0221 (5)	0.0204 (5)	0.0039 (4)	0.0077 (4)	0.0028 (4)
C8	0.0202 (5)	0.0172 (5)	0.0179 (5)	0.0001 (4)	0.0097 (4)	0.0012 (4)
C9	0.0154 (4)	0.0175 (5)	0.0162 (5)	0.0027 (4)	0.0090 (4)	−0.0003 (4)
C10	0.0202 (5)	0.0189 (5)	0.0188 (5)	−0.0012 (4)	0.0099 (4)	−0.0007 (4)
C11	0.0208 (5)	0.0274 (5)	0.0176 (5)	−0.0015 (4)	0.0073 (4)	−0.0032 (4)
C12	0.0221 (5)	0.0288 (6)	0.0156 (5)	0.0067 (4)	0.0097 (4)	0.0031 (4)
C13	0.0239 (5)	0.0204 (5)	0.0231 (5)	0.0038 (4)	0.0148 (4)	0.0040 (4)
C14	0.0187 (5)	0.0188 (5)	0.0205 (5)	−0.0003 (4)	0.0101 (4)	−0.0007 (4)

Geometric parameters (Å, º)

O1—C1	1.4266 (11)	C6—C7	1.3878 (14)
O1—H1	0.928 (18)	C6—H6	0.9500
N1—C2	1.4822 (12)	C7—C8	1.3926 (14)
N1—H11	0.907 (15)	C7—H7	0.9500
N1—H12	0.927 (15)	C8—H8	0.9500
C1—C3	1.5169 (13)	C9—C10	1.3903 (14)
C1—C2	1.5433 (13)	C9—C14	1.3974 (14)
C1—H1A	1.0000	C10—C11	1.3900 (14)
C2—C9	1.5133 (12)	C10—H10	0.9500
C2—H2	1.0000	C11—C12	1.3867 (15)
C3—C8	1.3910 (14)	C11—H11A	0.9500
C3—C4	1.3947 (14)	C12—C13	1.3877 (15)
C4—C5	1.3903 (14)	C12—H12A	0.9500
C4—H4	0.9500	C13—C14	1.3934 (14)
C5—C6	1.3881 (14)	C13—H13	0.9500
C5—H5	0.9500	C14—H14	0.9500
C1—O1—H1	105.9 (10)	C7—C6—H6	120.2
C2—N1—H11	107.7 (9)	C5—C6—H6	120.2
C2—N1—H12	108.9 (8)	C6—C7—C8	119.86 (9)
H11—N1—H12	106.3 (12)	C6—C7—H7	120.1
O1—C1—C3	111.09 (7)	C8—C7—H7	120.1
O1—C1—C2	107.56 (7)	C3—C8—C7	120.93 (9)
C3—C1—C2	112.40 (8)	C3—C8—H8	119.5
O1—C1—H1A	108.6	C7—C8—H8	119.5
C3—C1—H1A	108.6	C10—C9—C14	118.53 (9)

C2—C1—H1A	108.6	C10—C9—C2	120.14 (9)
N1—C2—C9	110.70 (8)	C14—C9—C2	121.33 (9)
N1—C2—C1	107.78 (7)	C11—C10—C9	121.00 (10)
C9—C2—C1	111.81 (8)	C11—C10—H10	119.5
N1—C2—H2	108.8	C9—C10—H10	119.5
C9—C2—H2	108.8	C10—C11—C12	120.15 (10)
C1—C2—H2	108.8	C10—C11—H11A	119.9
C8—C3—C4	118.71 (9)	C12—C11—H11A	119.9
C8—C3—C1	120.51 (9)	C13—C12—C11	119.52 (9)
C4—C3—C1	120.78 (9)	C13—C12—H12A	120.2
C5—C4—C3	120.50 (9)	C11—C12—H12A	120.2
C5—C4—H4	119.7	C12—C13—C14	120.29 (10)
C3—C4—H4	119.7	C12—C13—H13	119.9
C4—C5—C6	120.30 (9)	C14—C13—H13	119.9
C4—C5—H5	119.8	C13—C14—C9	120.50 (9)
C6—C5—H5	119.8	C13—C14—H14	119.7
C7—C6—C5	119.68 (9)	C9—C14—H14	119.7

O1—C1—C2—N1	54.01 (9)	C1—C3—C8—C7	178.98 (9)
C3—C1—C2—N1	176.61 (8)	C6—C7—C8—C3	0.44 (15)
O1—C1—C2—C9	175.90 (7)	N1—C2—C9—C10	−139.20 (9)
C3—C1—C2—C9	−61.50 (10)	C1—C2—C9—C10	100.61 (10)
O1—C1—C3—C8	−142.45 (9)	N1—C2—C9—C14	41.13 (12)
C2—C1—C3—C8	96.96 (10)	C1—C2—C9—C14	−79.06 (11)
O1—C1—C3—C4	37.40 (12)	C14—C9—C10—C11	−0.70 (14)
C2—C1—C3—C4	−83.18 (10)	C2—C9—C10—C11	179.61 (9)
C8—C3—C4—C5	0.49 (14)	C9—C10—C11—C12	−0.23 (15)
C1—C3—C4—C5	−179.37 (9)	C10—C11—C12—C13	0.73 (15)
C3—C4—C5—C6	0.34 (15)	C11—C12—C13—C14	−0.30 (15)
C4—C5—C6—C7	−0.79 (15)	C12—C13—C14—C9	−0.65 (15)
C5—C6—C7—C8	0.40 (15)	C10—C9—C14—C13	1.14 (14)
C4—C3—C8—C7	−0.88 (14)	C2—C9—C14—C13	−179.18 (9)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.93 (2)	1.89 (2)	2.813 (1)	172 (2)
N1—H11···O1^{ii}	0.91 (2)	2.38 (2)	3.178 (1)	148 (1)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*+1.