(1R,2R)-(+)-1,2-Diphenylethylenediamine

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Key indicators

Single-crystal X-ray study
$T = 180$ K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.082
Data-to-parameter ratio = 7.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of the title compound, $C_{14}H_{16}N_2$, has been determined at 180 (2) K in the non-centrosymmetric space group $P2_12_12_1$. The structure is formed by herring-bone-packed layers within which inter- and intramolecular N—H···N hydrogen bonds can be found, forming a one-dimensional infinite chain. Intermolecular N—H···π interactions are also present.

Comment
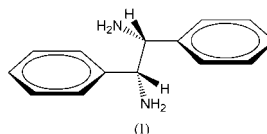
As part of our study devoted to the synthesis and characterization of novel chiral catalysts, we came across (1R,2R)-(+)-1,2-diphenylethylenediamine, (I), a bidentate chiral amine capable of forming chelates with transition metal cations (Jones *et al.*, 2003; Rouzaud *et al.*, 2003). Here we report the crystal structure, determined at 180 (2) K, of this chiral compound.

Compound (I) crystallizes in the orthorhombic non-centrosymmetric space group $P2_12_12_1$, with one whole molecule in the asymmetric unit (Fig. 1). Adjacent molecules of (I) are linked by a combination of inter- and intramolecular N—H···N hydrogen bonds (Table 2 and Fig. 2), forming a one-dimensional infinite chain which runs along the **a** direction (Fig. 3). Further intermolecular N—H···π interactions are also evident in the crystal structure [H2A···Cg^i = 2.61 (4) Å and N2—H2A···Cg^i = 138 (4)°, where Cg is the centroid of the C9–C14 ring; symmetry code: (i) $x - 1$, y, z] (Fig. 2). Although one could expect to find a similar interaction
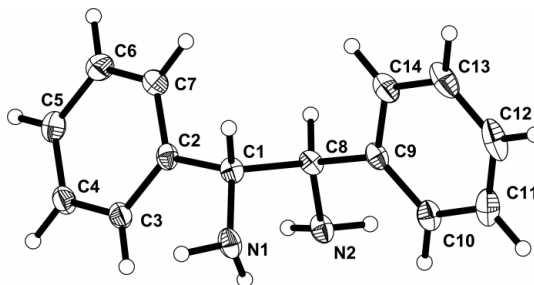
Figure 1
The molecular unit in (I), showing the labelling scheme for all non-H atoms. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres.
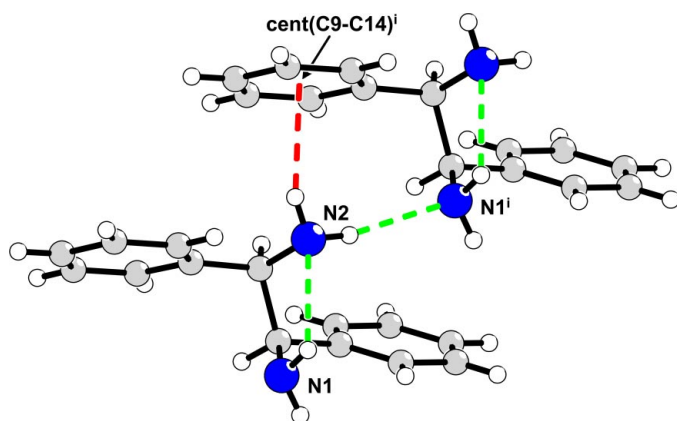
Figure 2
View, in detail, of the N—H···N intra- and intermolecular hydrogen bonds (dashed green lines) and the N—H···π interactions (red dashed lines) between adjacent molecules of (I). For hydrogen-bond details and symmetry code, see Table 2.
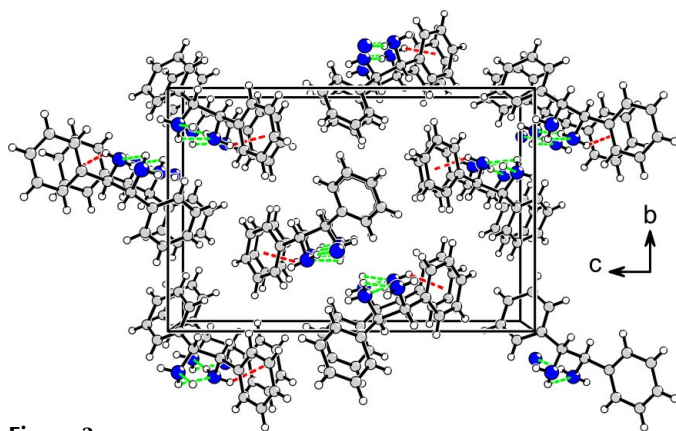

Figure 3
Perspective view of (I) along the **a** direction. Hydrogen bonds (see Table 2) are represented as green dashed lines, N—H···π interactions as red dashed lines.

between atom N1 and the neighbouring C2–C7 ring, the spatial arrangement of the molecules does not allow it. Individual molecules of (I) are stacked in a herring-bone manner, forming layers which pack in an *ABAB* fashion along the **b** direction (Fig. 3).

Experimental

(1*R*,2*R*)-(+)-1,2-Diphenylethylenediamine was purchased from Aldrich (99.99% purity) and used without further purification. Crystals suitable for X-ray diffraction analysis were obtained by recrystallization from methanol. ^{1}H NMR (CD$_3$OD): δ 3.95 (*s*, 1 H), 7.05–7.22 (*m*, 5 H). ^{13}C NMR (CD$_3$OD): δ 64.2 (CH), 128.5, 128.8, 129.5, 144.2 (Ph).

Crystal data

C$_{14}$H$_{16}$N$_2$	Mo $K\alpha$ radiation
$M_r = 212.29$	Cell parameters from 4851
Orthorhombic, $P2_12_12_1$	reflections
$a = 5.1447\ (1)$ Å	$\theta = 1.0$–$25.0°$
$b = 12.3264\ (4)$ Å	$\mu = 0.07$ mm^{-1}
$c = 18.5357\ (7)$ Å	$T = 180\ (2)$ K
$V = 1175.45\ (6)$ Å^3	Block, colourless
$Z = 4$	$0.23 \times 0.18 \times 0.12$ mm
$D_x = 1.200$ Mg m^{-3}	

Data collection

Nonius KappaCCD diffractometer	1148 reflections with $I > 2\sigma(I)$
Thin-slice ω and φ scans	$R_{int} = 0.056$
Absorption correction: multi-scan	$\theta_{max} = 25.0°$
(*SORTAV*; Blessing, 1995)	$h = -6 \rightarrow 6$
$T_{min} = 0.895$, $T_{max} = 0.992$	$k = -12 \rightarrow 14$
6085 measured reflections	$l = -21 \rightarrow 22$
1229 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.035$	$+ 0.2099P]$
$wR(F^2) = 0.082$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
1229 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
159 parameters	$\Delta\rho_{min} = -0.14$ e Å^{-3}
H atoms treated by a mixture of	Extinction correction: *SHELXL*97
independent and constrained	Extinction coefficient: 0.038 (6)
refinement	

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.456 (3)	C6—C7	1.380 (3)
N2—C8	1.463 (3)	C8—C9	1.516 (3)
C1—C2	1.524 (3)	C9—C10	1.387 (3)
C1—C8	1.551 (2)	C9—C14	1.394 (3)
C2—C3	1.390 (3)	C10—C11	1.390 (3)
C2—C7	1.394 (3)	C11—C12	1.378 (4)
C3—C4	1.390 (3)	C12—C13	1.372 (4)
C4—C5	1.379 (3)	C13—C14	1.385 (3)
C5—C6	1.392 (3)		
N1—C1—C2	116.33 (15)	N2—C8—C9	111.32 (16)
N1—C1—C8	108.93 (16)	N2—C8—C1	108.94 (15)
C2—C1—C8	109.41 (16)	C9—C8—C1	111.57 (16)
C3—C2—C7	117.77 (19)	C10—C9—C14	117.90 (19)
C3—C2—C1	123.08 (18)	C10—C9—C8	122.91 (18)
C7—C2—C1	119.13 (17)	C14—C9—C8	119.19 (18)
C4—C3—C2	120.46 (19)	C9—C10—C11	120.7 (2)
C5—C4—C3	121.18 (19)	C12—C11—C10	120.4 (2)
C4—C5—C6	118.9 (2)	C13—C12—C11	119.7 (2)
C7—C6—C5	119.8 (2)	C12—C13—C14	120.0 (2)
C6—C7—C2	121.85 (19)	C13—C14—C9	121.2 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···N2	0.916 (17)	2.34 (2)	2.832 (2)	113.1 (16)
N2—H2B···N1^i	0.927 (18)	2.346 (18)	3.249 (2)	164.3 (17)

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

H atoms bound to C atoms were placed in calculated positions and allowed to ride during subsequent refinement, with $U_{iso}(H) = 1.2U_{eq}(C)$. The NH$_2$ H atoms were located from difference Fourier maps and refined successfully. A total of 801 Friedel pairs were merged and not used as independent data. The corresponding Flack (1983) parameter was found to be meaningless and was omitted.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXTL* (Bruker, 2001); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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