

(R)-(+)-2,2'-Diamino-1,1'-binaphthyl**Matthew D. Jones,* Filipe A. Almeida Paz, John E. Davies and Brian F. G. Johnson**

Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England

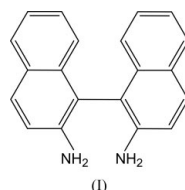
Correspondence e-mail: mdj22@cam.ac.uk

Key indicatorsSingle-crystal X-ray study
 $T = 180$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.036
 wR factor = 0.100
Data-to-parameter ratio = 9.8For 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, $\text{C}_{20}\text{H}_{16}\text{N}_2$, has been determined at 180 (2) K in the chiral space group $P4_32_12$. The structure is described by a herring-bone close-packing, along the **a** and **b** directions, of layers within which intermolecular $\text{N}-\text{H}\cdots\pi$ and $\text{C}-\text{H}\cdots\pi$ interactions can be found.

Comment

We have been focusing our research on the use of amines which can lead to the synthesis of chiral metal complexes with applications, for example, as catalysts in asymmetric hydrogenation processes (Jones *et al.*, 2003*a,b,c*; Raynor *et al.*, 2000). As part of our study, we came across (*R*)-2,2'-diamino-1,1'-binaphthyl, (I), an interesting bidentate chiral amine capable of forming chelates with transition metal centres (Mikami *et al.*, 2002; Mikami & Aikawa, 2002; Jones *et al.*, 2003*a*). Gridunova *et al.* (1982) have investigated the structure of racemic 2,2'-diamino-1,1'-binaphthyl. Here we report the crystal structure, determined at 180 (2) K, of the pure *R* form.



Compound (I) crystallizes in the tetragonal chiral space group $P4_32_12$, with the origin located at 2_112 and the asymmetric unit containing only half of the molecular unit (Fig. 1). Adjacent molecules of (I) are linked by a combination of intermolecular $\text{N}-\text{H}\cdots\pi$ and $\text{C}-\text{H}\cdots\pi$ interactions [$\text{H}1\text{B}\cdots\text{Cg}^i = 2.60$ (3) Å and $\text{N}1-\text{H}1\text{B}\cdots\text{Cg}^i = 166$ (3)°, $\text{H}5\cdots\text{Cg}^{ii} = 2.68$ Å and $\text{C}5-\text{H}5\cdots\text{Cg}^{ii} = 159$ °, where Cg is the centroid of the $\text{C}4-\text{C}9$ aromatic ring; symmetry codes: (i) $y, -1 + x, -z$; (ii) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{4} - z$] (see Fig. 2). Although one could expect to find a similar $\text{N}-\text{H}\cdots\pi$ interaction between the $\text{N}1-\text{H}1\text{A}$ bond and a neighbouring aromatic ring, the spatial arrangement of the molecules does not allow it. Individual molecules of (I) are arranged in the **c** direction in a way that leads to a herring-bone packing manner (Fig. 3).

Experimental

(*R*)-(+)-2,2'-Diamino-1,1'-binaphthyl was purchased from Aldrich (99.5% purity) and used without further purification. Crystals suitable for X-ray diffraction analysis were obtained by recrystallization from methanol.

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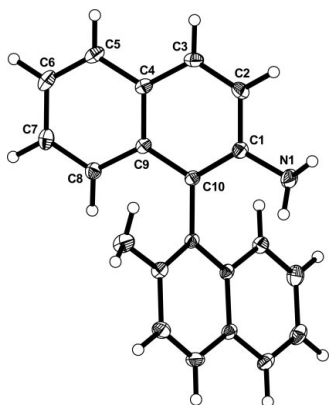


Figure 1

The molecular structure of (I), showing the labelling scheme for all non-H atoms in the asymmetric unit. Displacement ellipsoids are drawn at the 30% probability level.

Crystal data

$C_{20}H_{16}N_2$
 $M_r = 284.35$
 Tetragonal, $P4_32_12$
 $a = 7.0388$ (2) Å
 $c = 30.0684$ (8) Å
 $V = 1489.73$ (7) Å³
 $Z = 4$
 $D_x = 1.268$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 4522 reflections
 $\theta = 1.0$ – 27.5°
 $\mu = 0.08$ mm⁻¹
 $T = 180$ (2) K
 Block, colourless
 $0.46 \times 0.46 \times 0.23$ mm

Data collection

Nonius KappaCCD diffractometer
 Thin-slice ω and φ scans
 Absorption correction: multi-scan (SORTAV; Blessing, 1995)
 $T_{\min} = 0.944$, $T_{\max} = 0.983$
 4236 measured reflections
 1635 independent reflections

1455 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -9 \rightarrow 9$
 $k = -6 \rightarrow 9$
 $l = -39 \rightarrow 39$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.100$
 $S = 1.02$
 1061 reflections
 108 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.37P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N1—C1	1.378 (2)	C5—C6	1.363 (3)
C1—C10	1.393 (2)	C6—C7	1.409 (3)
C1—C2	1.423 (2)	C7—C8	1.374 (2)
C2—C3	1.355 (2)	C8—C9	1.422 (2)
C3—C4	1.417 (2)	C9—C10	1.433 (2)
C4—C5	1.419 (2)	C10—C10 ⁱⁱⁱ	1.496 (3)
C4—C9	1.426 (2)		
N1—C1—C10	121.72 (15)	C5—C6—C7	119.91 (16)
N1—C1—C2	117.93 (15)	C8—C7—C6	120.63 (17)
C10—C1—C2	120.30 (15)	C7—C8—C9	121.05 (17)
C3—C2—C1	121.25 (16)	C8—C9—C4	117.82 (14)
C2—C3—C4	120.61 (16)	C8—C9—C10	122.26 (14)
C3—C4—C5	121.36 (16)	C4—C9—C10	119.91 (15)
C3—C4—C9	119.09 (15)	C1—C10—C9	118.79 (14)
C5—C4—C9	119.55 (16)	C1—C10—C10 ⁱⁱⁱ	119.46 (14)
C6—C5—C4	121.02 (16)	C9—C10—C10 ⁱⁱⁱ	121.58 (15)

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

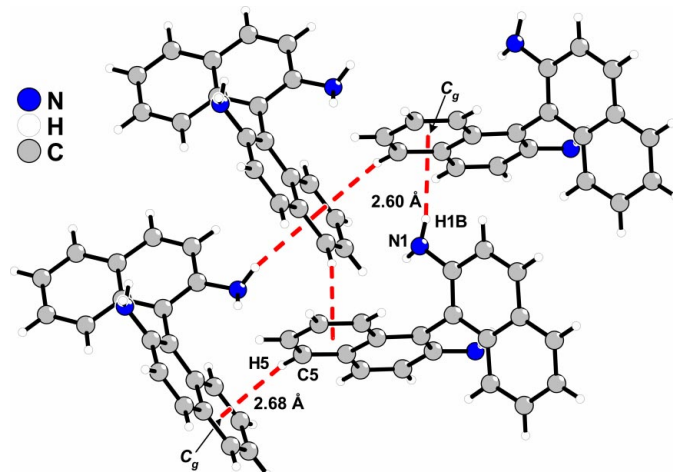


Figure 2

View of the intermolecular N—H... π and C—H... π interactions (dashed red lines) between adjacent molecules of (I). C_g is the centroid of the C4—C9 aromatic ring.

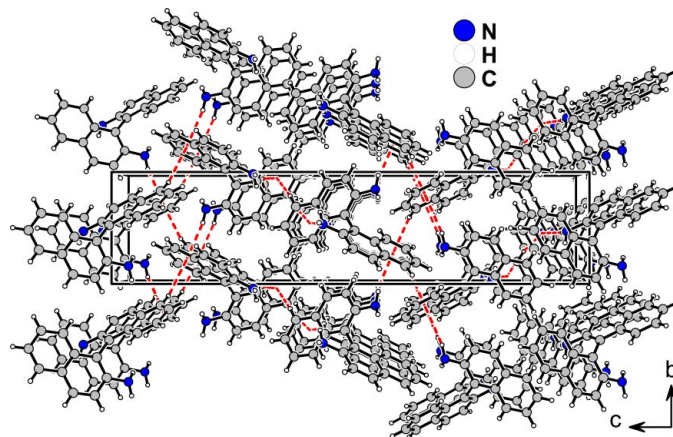


Figure 3

Perspective view of (I) along the a axis. N—H... π and C—H... π interactions are represented as dashed red lines.

All H atoms bound to C atoms were placed in calculated positions and allowed to ride during subsequent refinement, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The NH₂ H atoms were located in a difference Fourier map and refined independently. A total of 574 Friedel pairs have been 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: *SIR92* (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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