

**(S)-(-)-1,1'-Bi-2-naphthol dimethylformamide sesquisolvate****Ji-Xin Yuan,<sup>a</sup> Xin-Yuan Song<sup>b</sup> and Seik Weng Ng<sup>c\*</sup>**<sup>a</sup>School of Chemistry and Materials Science, Wenzhou University, Wenzhou 325027, People's Republic of China, <sup>b</sup>College of Chemistry and Chemical Engineering, Donghua University, Shanghai 200051, People's Republic of China, and <sup>c</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

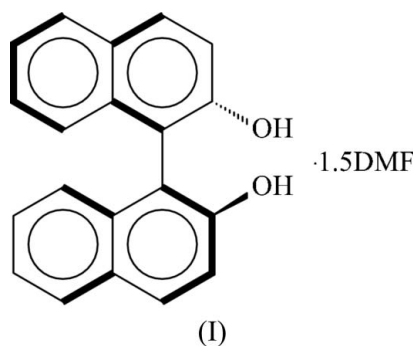
Correspondence e-mail: seikweng@um.edu.my

**Key indicators**Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
Disorder in solvent or counterion  
 $R$  factor = 0.076  
 $wR$  factor = 0.193  
Data-to-parameter ratio = 8.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the crystal structure of the title compound,  $\text{C}_{20}\text{H}_{14}\text{O}_2 \cdot 1.5\text{C}_3\text{H}_7\text{N O}$ , one of the hydroxyl groups forms a hydrogen bond to the dimethylformamide (DMF) molecule that lies on a general position and the other a hydrogen bond to the DMF molecule that lies on a twofold rotation axis. The naphthyl residues are aligned at  $75.8(1)^\circ$  with respect to each other.

**Comment**

The preceding paper (Yuan *et al.*, 2005) reports the structure of racemic 1,1'-bi-2-naphthol DMF sesquisolvate. In the title optically active *S*-form, (I) (Fig. 1), the two aromatic residues enclose a dihedral angle of  $75.8(1)^\circ$ . One of the hydroxy groups forms a hydrogen bond to the ordered DMF (which lies on a general position) and the other one to the disordered DMF (which lies on a twofold rotation axis) (Table 1).



The hydrogen bonding is similar to that found in the racemic solvate (Yuan *et al.*, 2005). However, the packing is somewhat more efficient, as noted from the density ( $1.235 \text{ Mg m}^{-3}$ ) compared with that of the racemic solvate ( $1.222 \text{ Mg m}^{-3}$ ). The angle between the two aromatic systems is similar to that found in the anhydrous compound, which crystallizes in space group *P*32 (Toda *et al.*, 1997). The structure of the anhydrous *R*-(+)-enantiomer has also been reported (Mori *et al.*, 1993).

**Experimental**

*S*-(-)-1,1'-Bi-2-naphthol (0.29 g, 1 mmol) was dissolved in a mixed-solvent system of water (5 ml) and dimethylformamide (5 ml). This solution was added to an ethanol solution (10 ml) of 2-aminopyrimidine (0.19 g, 2 mmol). Evaporation of the solvent over several weeks gave colourless block-shaped crystals of (I).

Received 20 September 2005

Accepted 22 September 2005

Online 28 September 2005

Crystal data

C<sub>20</sub>H<sub>14</sub>O<sub>2</sub>·1.5C<sub>3</sub>H<sub>7</sub>NO  
*M<sub>r</sub>* = 395.96  
 Tetragonal, *P*4<sub>3</sub>2<sub>1</sub>2  
*a* = 8.8430 (5) Å  
*c* = 54.486 (3) Å  
*V* = 4260.7 (3) Å<sup>3</sup>  
*Z* = 8  
*D<sub>x</sub>* = 1.235 Mg m<sup>-3</sup>

Mo *K*α radiation  
 Cell parameters from 4002 reflections  
 $\theta = 2.3\text{--}23.0^\circ$   
 $\mu = 0.08\text{ mm}^{-1}$   
*T* = 295 (2) K  
 Block, colourless  
 0.36 × 0.20 × 0.19 mm

Data collection

Bruker APEX CCD area-detector diffractometer  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: none  
 22486 measured reflections  
 2335 independent reflections

2240 reflections with *I* > 2σ(*I*)  
*R*<sub>int</sub> = 0.046  
 $\theta_{\text{max}} = 25.0^\circ$   
*h* = -10 → 9  
*k* = -10 → 10  
*l* = -64 → 64

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.076  
*wR* (*F*<sup>2</sup>) = 0.193  
*S* = 1.37  
 2335 reflections  
 287 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0793P)^2 + 1.8739P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.18\text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.25\text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ··· <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> — <i>H</i> ··· <i>A</i>
O1—H1···O3	0.82	1.87	2.681 (5)	171
O2—H2···O4	0.82	2.04	2.820 (5)	158

One DMF molecule is disordered over a twofold rotation axis. A number of restraints were imposed on this molecule, as follows: C24—O4 = 1.25 (1), C24—N2 = 1.35 (1), N2—C25 = N2—C26 = 1.45 (1), O4···C25 = 2.71 (1), C24···C25 = C24···C26 = 2.43 (2) and C25···C26 = 2.51 (2) Å. The displacement parameters of these atoms were restrained to an approximate isotropic behaviour; furthermore, these atoms were restrained to lie in a common plane. H atoms were positioned geometrically (O—H = 0.82, C—H<sub>aromatic</sub> = 0.93 and C—H<sub>methyl</sub> = 0.96 Å), and were included in the refinement in the riding-model approximation, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C,O), or 1.5*U*<sub>eq</sub>(C) for methyl groups. In the absence of significant anomalous scattering effects, Friedel pairs were merged. The absolute configuration is known from the synthesis.

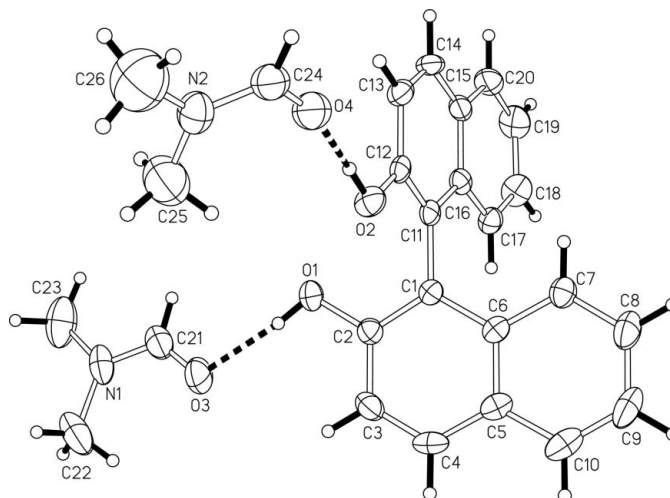


Figure 1

A plot of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radii. Dashed lines indicate hydrogen bonds. Only one disorder component is shown.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINTE* (Bruker, 2003); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank Wenzhou Normal College, Donghua University and the University of Malaya for supporting this work.

References

- Bruker (2003). *SAINTE* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Mori, K., Masuda, Y. & Kashino, S. (1993). *Acta Cryst.* **C49**, 1224–1227.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Toda, F., Tanaka, K., Miyamoto, H., Koshima, H., Miyahara, I. & Hirotsu, K. (1997). *J. Chem. Soc. Perkin Trans. 2*, pp. 1877–1885.
- Yuan, J.-X., Song, X.-Y. & Ng, S. W. (2005). *Acta Cryst.* **E61**, o3457–o3458.