

Two crystalline modifications of
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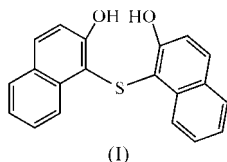
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The title compound, $C_{20}H_{14}O_2S$, has been obtained in two monoclinic forms, which differ in their unit-cell dimensions, compactness of packing and conformation. Pairwise association of molecules occurs *via* complementary $O-H\cdots O$ hydrogen bonding.

Comment

1,1'-Thiobis(2-naphthol), (I), has been obtained in two crystalline forms (Fig. 1, and Tables 1 and 3) with distinctly different unit cells.



At first sight, form (Ia), with a short *a* axis, appears to exhibit a more compact packing than does form (Ib), with a short *b* axis, as is depicted in Figs. 2 and 3. However, simulated radial distribution functions of the two structures indicate a larger number of intermolecular contacts in the 3.5–5.0 Å range, suggesting that (Ib) possesses a slightly more compact structure. Despite this, four contacts of 3.349 (2)–3.490 (2) Å occur between atom S1 and atoms C12–C15 in the neighboring molecule at (*x* + 1, *y*, *z*) in (Ia), whereas in (Ib), atom S1 forms contacts with only atom C5 in the molecule at (*x*, *y* + 1, *z*), at a distance of 3.344 (2) Å. These $S\cdots C$ contacts propagate parallel to *a* in (Ia) and parallel to *b* in (Ib).

Additionally, besides the $H1\cdots O2$ hydrogen bond that is seen in both forms (Tables 2 and 4), the pattern of potential interactions of atom H2 with its surroundings differs between (Ia) and (Ib). In the former, there is an intermolecular contact of 2.46 (3) Å with atom $O1^{ii}$ [$O2-H2\cdots O1^{ii} = 134 (3)^\circ$; symmetry code: (ii) $-x + 1, -y, -z$] and an intramolecular contact of 2.41 (2) Å with atom S1 [$O2-H2\cdots S1 = 125 (2)^\circ$], while in the latter, the closest contacts are both intramolecular

[$H2\cdots O1 = 2.50 (2) \text{ \AA}$ and $O2-H2\cdots O1 = 104 (2)^\circ$; $H2\cdots S1 = 2.40 (2) \text{ \AA}$ and $O2-H2\cdots S1 = 126 (2)^\circ$]. In both instances, the $H2\cdots S1$ contacts are comparable to previously reported $O-H\cdots S$ hydrogen bonds (Allen *et al.*, 1997). The torsional orientation of the $O2-H2$ bond in both forms suggests a weak bifurcated hydrogen bond.

In both forms, the naphthyl groups are planar to within 0.004–0.01 Å, with dihedral angles between the mean planes of $100.0 (1)^\circ$ for (Ia) and $96.5 (1)^\circ$ in (Ib). Modest differences in the overall conformations of the molecule between the two forms are also seen in the $C2-C1-S1-C11$ and $C12-C11-S1-C1$ torsion angles, which are $-64.8 (2)$ and $112.5 (2)^\circ$, respectively, in (Ia) and $-60.5 (2)$ and $105.6 (2)^\circ$, respectively, in (Ib).

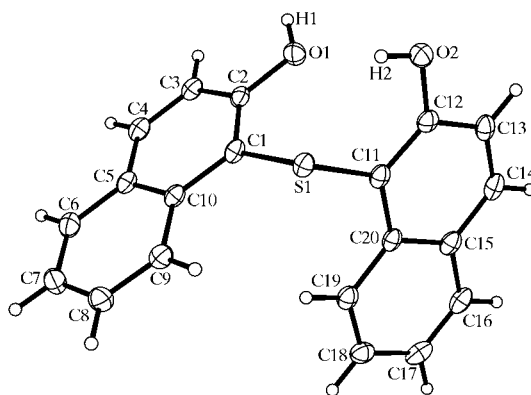


Figure 1

A perspective view of (Ib). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn arbitrarily small for clarity.

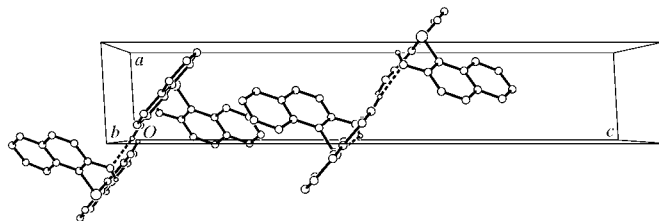


Figure 2

The molecular packing for (Ia), viewed down the *b* axis.

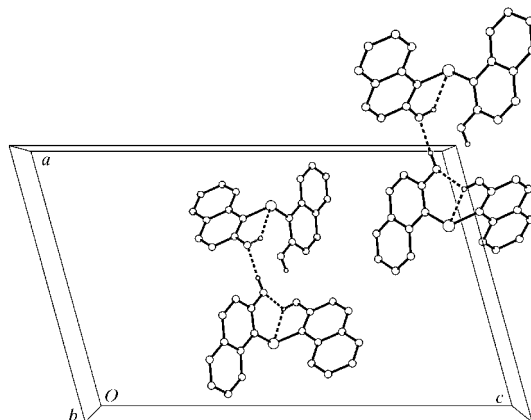


Figure 3

The molecular packing for (Ib), viewed down the *b* axis.

Experimental

Form (Ia) was obtained in an attempt to grow crystals of $\text{Fe}\{\eta^5\text{-C}_5\text{H}_4\text{P}[-\text{OC}_{10}\text{H}_6(\mu\text{-S})\text{C}_{10}\text{H}_6\text{O-}]\}$ (Punji *et al.*, 2007) from a mixture of dichloromethane and petroleum ether. Form (Ib) was obtained in an attempt to crystallize $\{[-\text{OC}_{10}\text{H}_6(\mu\text{-S})\text{C}_{10}\text{H}_6\text{O-}]\text{P}(=\text{S})\}_2\{\mu\text{-}[-\text{OC}_{10}\text{H}_6(\mu\text{-S})\text{C}_{10}\text{H}_6\text{O-}]\}$ (Punji *et al.*, 2007) in a similar fashion. Both were additionally characterized by comparison of their melting points with that of an authentic sample.

Form (Ia)

Crystal data

$\text{C}_{20}\text{H}_{14}\text{O}_2\text{S}$ $V = 1464.7(3) \text{ \AA}^3$
 $M_r = 318.37$ $Z = 4$
 Monoclinic, $P2_1/n$ Mo $K\alpha$ radiation
 $a = 4.8053(6) \text{ \AA}$ $\mu = 0.23 \text{ mm}^{-1}$
 $b = 11.420(1) \text{ \AA}$ $T = 100(2) \text{ K}$
 $c = 26.732(3) \text{ \AA}$ $0.22 \times 0.10 \times 0.07 \text{ mm}$
 $\beta = 93.181(2)^\circ$

Data collection

Bruker SMART APEX CCD area-detector diffractometer 12389 measured reflections
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002) 3339 independent reflections
 $T_{\min} = 0.953$, $T_{\max} = 0.987$ 2472 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$ H atoms treated by a mixture of independent and constrained refinement
 $wR(F^2) = 0.106$ $\Delta\rho_{\text{max}} = 0.37 \text{ e \AA}^{-3}$
 $S = 1.01$ $\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$
 3339 reflections
 216 parameters

Table 1

Selected geometric parameters (\AA , $^\circ$) for (Ia).

S1—C11	1.780 (2)	S1—C1	1.780 (2)
C11—S1—C1	104.60 (9)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$) for (Ia).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O1—H1 \cdots O2 ⁱ	0.83 (3)	2.00 (3)	2.826 (2)	171 (3)

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

Form (Ib)

Crystal data

$\text{C}_{20}\text{H}_{14}\text{O}_2\text{S}$ $V = 1460.59(15) \text{ \AA}^3$
 $M_r = 318.37$ $Z = 4$
 Monoclinic, $P2_1/n$ Mo $K\alpha$ radiation
 $a = 13.6508(9) \text{ \AA}$ $\mu = 0.23 \text{ mm}^{-1}$
 $b = 5.2192(3) \text{ \AA}$ $T = 100(2) \text{ K}$
 $c = 21.265(1) \text{ \AA}$ $0.20 \times 0.09 \times 0.05 \text{ mm}$
 $\beta = 105.409(1)^\circ$

Data collection

Bruker SMART APEX CCD area-detector diffractometer 23840 measured reflections
 Absorption correction: multi-scan (SADABS; Sheldrick, 2007) 3330 independent reflections
 $T_{\min} = 0.922$, $T_{\max} = 0.988$ 2828 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$ H atoms treated by a mixture of independent and constrained refinement
 $wR(F^2) = 0.091$ $\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$
 $S = 1.09$ $\Delta\rho_{\text{min}} = -0.31 \text{ e \AA}^{-3}$
 3330 reflections
 216 parameters

Table 3

Selected geometric parameters (\AA , $^\circ$) for (Ib).

S1—C11	1.784 (2)	S1—C1	1.787 (2)
C11—S1—C1	102.73 (9)		

Table 4

Hydrogen-bond geometry (\AA , $^\circ$) for (Ib).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O1—H1 \cdots O2 ⁱ	0.86 (3)	1.90 (3)	2.7581 (19)	175 (3)

Symmetry code: (i) $-x + 2, -y + 1, -z + 2$.

H atoms attached to C atoms were placed in calculated positions ($\text{C—H} = 0.95 \text{ \AA}$) and included as riding contributions, with $U_{\text{iso}}(\text{H})$ values of $1.2U_{\text{eq}}$ of the attached C atoms. H atoms attached to O atoms were refined with isotropic displacement parameters.

For form (Ia), data collection: SMART (Bruker, 2000); cell refinement: SAINT-Plus (Bruker, 2004); data reduction: SAINT-Plus; molecular graphics: SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXTL. For form (Ib), data collection: APEX2 (Bruker, 2006); cell refinement: APEX2; data reduction: SAINT-Plus (Bruker, 2006); molecular graphics: APEX2; software used to prepare material for publication: APEX2. For both compounds, program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FA3098). Services for accessing these data are described at the back of the journal.

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