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#### Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma$ (C–C) = 0.008 Å  
R factor = 0.068  
wR factor = 0.160  
Data-to-parameter ratio = 10.8

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

## S-Methyl *trans-cis*- $\beta$ -N-(2-hydroxynaphthyl)methylenedithiocarbazate

In the title compound, C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>OS<sub>2</sub>, the whole molecule is nearly planar. The molecules are linked by N–H...S hydrogen bonds between the amino group and the thione S atoms, forming molecular chains along the *a* direction.

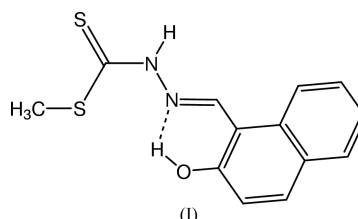
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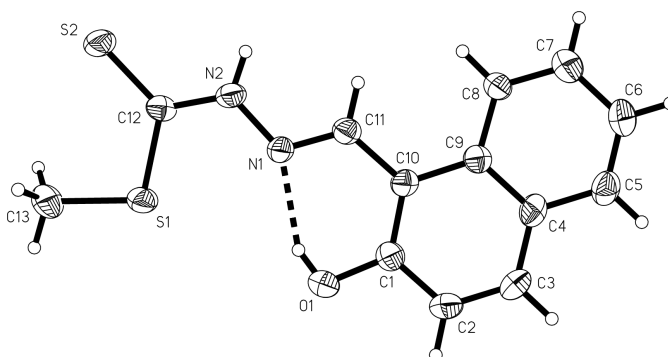
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#### Comment

The study of dithiocarbazate derivatives and their metal complexes is prompted by their potential as biologically active agents (Tarafder, Saravanan *et al.*, 2001; Tarafder, Kasbollah *et al.*, 2001). The possible conformations formed in dithiocarbazate compounds and in their metal complexes are also of interest. Our attempts to prepare a new dithiocarbazate ligand led us to the title compound, (I). An X-ray structure analysis of (I) was undertaken in order to elucidate its conformation.



The bond lengths and angles in the title compound, (I) (Fig. 1), are within normal ranges (Allen *et al.*, 1987). The C11–N1, N1–N2 and C12–S2 bond lengths of 1.284 (6), 1.368 (5) and 1.665 (5) Å, respectively, are typical of Schiff base compounds of the dithiocarbazate system (S1/S2/C12/N2), *e.g.* *S*-methyl *N*<sup>β</sup>-(4-nitrobenzal)methylenedithiocarbazate [the corresponding values are 1.265 (4), 1.376 (3) and 1.661 (2) Å, respectively; Duan *et al.*, 1997]. The title compound is in the *trans-cis* configuration, as was observed in other dithiocarbazate analogues, such as *S*-methyl dithiocarbazate (Mattes & Weber, 1980) and *S*-benzyl dithiocarbazate (Shanmuga Sundara Raj *et al.*, 2000).



**Figure 1**

The molecular structure of (I), with 50% probability displacement ellipsoids.

The whole molecule of the title compound (Fig. 1) is nearly planar, with a dihedral angle of  $3.1(1)^\circ$  between the dithiocarbazate (S1/S2/C12/N2) and naphthalene (C1–C10) systems. The planarity is due to the  $\pi$ -conjugation of the N1=C11 and N1–N2 joining the two systems. Atom C13 is displaced by  $0.022(2)$  Å from the dithiocarbazate plane, while the hydroxy atom O1 deviates by  $0.025(5)$  Å from the naphthalene plane.

In the title structure, there is an intramolecular O1–H1A $\cdots$ N1 (Table 2) hydrogen bond, forming a six-membered N1–C11–C10–C1–O1–H1A ring. This interaction also contributes to the planarity of the title compound. The molecules are linked by three N–H $\cdots$ S hydrogen bonds (Table 2) between the amino group and thione S atom, forming a three-dimensional molecular network. Fig. 2 shows the packing diagram of (I), viewed down the *a* axis, showing the molecular chains along the *a* direction.

## Experimental

S-Methyldithiocarbazate (0.176 g, 0.01 mol) in ethanol was added to 20 ml of ethanol solution containing 2-hydroxynaphthaldehyde (0.172 g, 0.01 mol). The solution was stirred with a magnetic stirrer at 328 K for about 15 min. The resulting yellow precipitate was filtered and washed with ethanol followed by petroleum ether. Single crystals were grown by slow evaporation from a dimethyl sulfoxide solution.

### Crystal data

C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> OS <sub>2</sub>	Mo K $\alpha$ radiation
$M_r = 276.37$	Cell parameters from 4198 reflections
Orthorhombic, $P2_12_12_1$	$\theta = 2.7\text{--}28.3^\circ$
$a = 5.1608(1)$ Å	$\mu = 0.41$ mm <sup>-1</sup>
$b = 9.4909(2)$ Å	$T = 293(2)$ K
$c = 25.8492(7)$ Å	Slab, yellow
$V = 1266.11(5)$ Å <sup>3</sup>	$0.50 \times 0.36 \times 0.18$ mm
$Z = 4$	
$D_x = 1.450$ Mg m <sup>-3</sup>	

### Data collection

Siemens SMART CCD area-detector diffractometer	1819 independent reflections
$\omega$ scans	1354 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.098$
$T_{\text{min}} = 0.822$ , $T_{\text{max}} = 0.930$	$\theta_{\text{max}} = 28.4^\circ$
7639 measured reflections	$h = -6 \rightarrow 6$
	$k = -12 \rightarrow 9$
	$l = -29 \rightarrow 34$

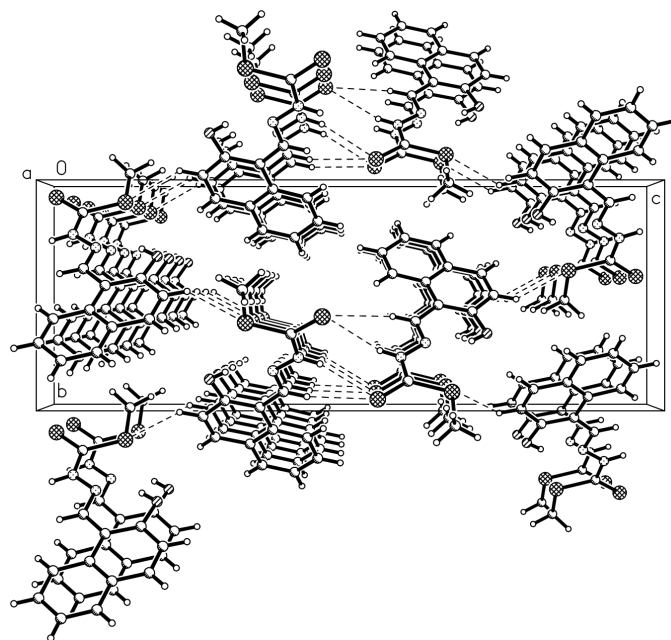
### Refinement

Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.0835P)^2]$
$wR(F^2) = 0.160$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1819 reflections	$\Delta\rho_{\text{max}} = 1.14$ e Å <sup>-3</sup>
168 parameters	$\Delta\rho_{\text{min}} = -0.66$ e Å <sup>-3</sup>

**Table 1**

Selected interatomic distances (Å).

S1–C12	1.751(5)	N1–C11	1.284(6)
S1–C13	1.786(6)	N1–N2	1.368(5)
S2–C12	1.664(5)	N2–C12	1.325(6)



**Figure 2**

Packing diagram of the title compound, viewed down the *a* axis. The dashed lines denote the N–H $\cdots$ S hydrogen bonds.

**Table 2**

Hydrogen-bonding geometry (Å, °).

D–H $\cdots$ A	D–H	H $\cdots$ A	D $\cdots$ A	D–H $\cdots$ A
O1–H1A $\cdots$ N1	0.79(6)	1.90(5)	2.634(5)	153(6)
C11–H11 $\cdots$ S2 <sup>i</sup>	0.93	2.94	3.780(5)	150
N2–H2A $\cdots$ S2 <sup>i</sup>	0.86	2.64	3.482(4)	165
C2–H2 $\cdots$ S1 <sup>ii</sup>	0.93	2.90	3.573(6)	130

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

The absolute configuration could not be determined, and Friedel pairs were merged. After location in a difference map, all H atoms, except the hydroxy H atom, were fixed geometrically and allowed to ride on the parent C or N atoms, with C–H = 0.97 Å and N–H = 0.89 Å.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 1990).

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