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# Difluoro[1-(1-naphthyliminomethyl)-2-naphtholato-*N*,*O*]boron

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.044
*wR* factor = 0.122
Data-to-parameter ratio = 16.0

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



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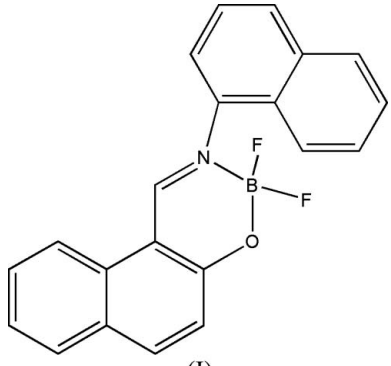
The title compound, $C_{21}H_{14}BF_2NO$, was synthesized by the reaction of 3-[(*E*)-(naphthalen-1-ylimino)methyl]naphthalen-2-ol, diisopropylethylamine and boron trifluoride etherate. The mean planes of the two naphthalene systems make a dihedral angle of 71.97 (4)°. The crystal packing is stabilized by π–π stacking interactions and van der Waals forces.

## Comment

The chelates involving boron trifluoride and organic ligands have attracted attention owing to their unique photoelectronic properties. For instance, the boron dipyrromethenes and dioxaborines with β-diketonates can be used in photodynamic therapy (Halik *et al.*, 2003) and utilized as laser dyes (Assor *et al.*, 1998), molecular probes (Gabe *et al.*, 2004) and nonlinear optical materials (Gorman *et al.*, 2004). This prompted us to prepare the title compound, (I), which is the $BF_2$ chelate of 3-[(*E*)-(naphthalen-1-ylimino)methyl]naphthalen-2-ol. We report here the crystal structure of (I).




(I)

In the title molecule (Fig. 1), all bond lengths and angles show normal values (Allen *et al.*, 1987). The mean planes of the C2–C11 and C12–C21 naphthalene systems make a dihedral angle of 71.97 (4)°. The relatively short intermolecular C···C distances C8···C8$^{i}$ of 3.522 (3) Å and C14···C16$^{ii}$ of 3.480 (3) Å [symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $2-x, -y, 1-z$] indicate the presence of π–π stacking interactions, which contribute to the stabilization of the crystal packing (Fig. 2) along with van der Waals forces.

## Experimental

At room temperature, the Schiff base 3-[(*E*)-(naphthalen-1-ylimino)methyl]naphthalen-2-ol (0.5 mmol) was dissolved in anhydrous $CH_2Cl_2$ (30 ml); diisopropylethylamine (5 mmol) and boron trifluoride etherate (10 mmol) were then added. The resulting solu-

tion was stirred for 24 h under an $N_2$ flow. The mixture was washed with water (2 × 50 ml), and the organic layer was dried over anhydrous sodium sulfate. Purification by column chromatography on silica eluting with $CH_2Cl_2$/petroleum ether (1:2) gave the title chelate in 86% yield as a crystalline solid. Suitable crystals were obtained by evaporation of an acetone/water (1:1) mixed solution (m.p. 511–513 K).

*Crystal data*

| | |
|---|---|
| $C_{21}H_{14}BF_2NO$ | $Z = 4$ |
| $M_r = 345.14$ | $D_x = 1.381$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 10.195$ (2) Å | $\mu = 0.10$ mm$^{-1}$ |
| $b = 15.524$ (3) Å | $T = 293$ (2) K |
| $c = 10.498$ (2) Å | Prism, colourless |
| $\beta = 92.28$ (3)° | 0.33 × 0.18 × 0.11 mm |
| $V = 1660.1$ (6) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 15916 measured reflections |
| $\omega$ scans | 3771 independent reflections |
| Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) | 2321 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.956$, $T_{max} = 0.990$ | $R_{int} = 0.033$ |
| | $\theta_{max} = 27.5°$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.1252P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2) = 0.122$ | $\Delta\rho_{max} = 0.31$ e Å$^{-3}$ |
| $S = 1.06$ | $\Delta\rho_{min} = -0.22$ e Å$^{-3}$ |
| 3771 reflections | Extinction correction: *SHELXL97* |
| 236 parameters | Extinction coefficient: 0.0083 (14) |
| H-atom parameters constrained | |

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

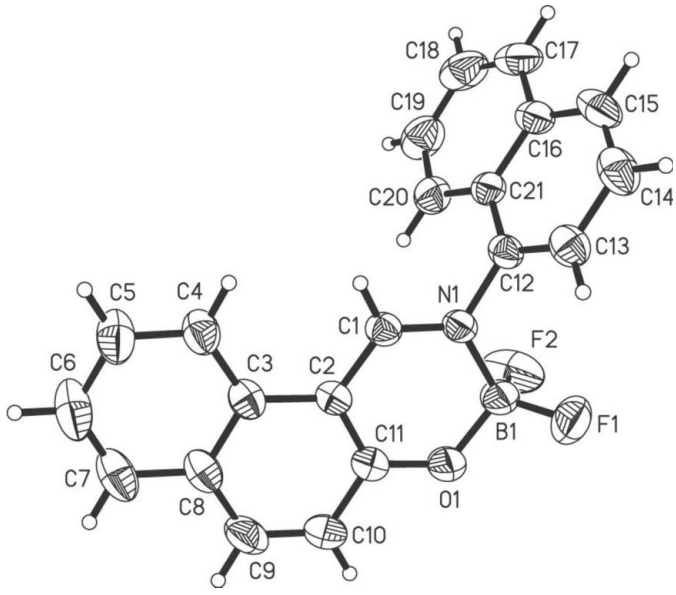



**Figure 1**
View of (I), showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. H atoms are represented by spheres of arbitrary radii.

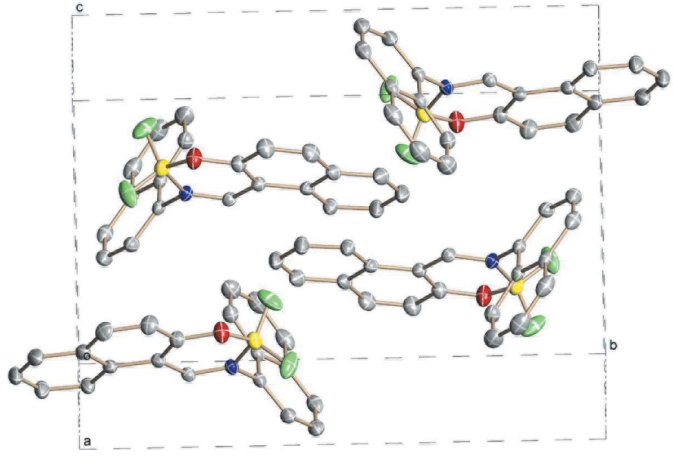



**Figure 2**
The molecular packing. H atoms have been omitted for clarity.

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