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#### Key indicators

Single-crystal X-ray study  
T = 298 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
R factor = 0.043  
wR factor = 0.110  
Data-to-parameter ratio = 14.5

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

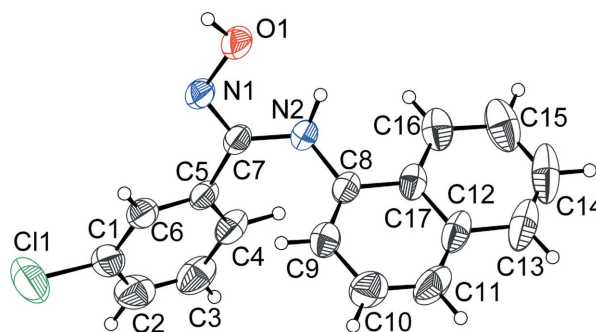
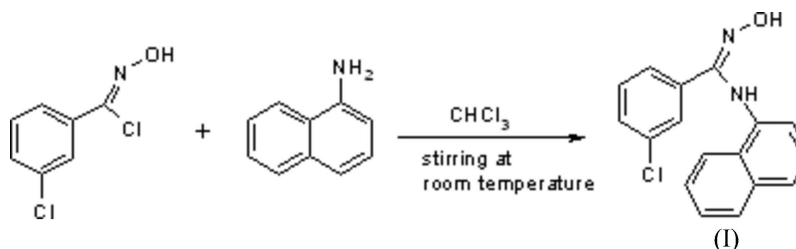
## 3-Chloro-*N'*-hydroxy-*N*-(1-naphthyl)benzene- carboximidamide

The molecule of the title compound,  $\text{C}_{17}\text{H}_{13}\text{ClN}_2\text{O}$ , adopts a *cis* configuration with respect to the  $\text{C}=\text{N}$  bond. The crystal structure features  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonding.

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#### Comment

Amidoximes have been of great interest for many years. They have proved to be biologically active compounds in terms of antituberculostatic, antithrombotic and vasodilating, anti-malarial, antidepressive and alpha-adrenergic activities (Nieves-Neira *et al.*, 1999). They are also used as intermediates in the synthesis of various types of heterocyclic compounds, *e.g.* oxadiazoles (Yu *et al.*, 2005) and oxadiazines (Dürüst, 1998). They are highly reactive compounds and have been extensively used as absorbents for uranium (Zhang *et al.*, 2005),  $\text{Cu}^{2+}$  ions (Kondo *et al.*, 1999) and vanadium (Seko *et al.*, 2005) in sea-water. An amidoxime-based chelating resin has been prepared by Zohuriaan-Mehr *et al.* (2004) and exhibited high sorption capacity towards metal ions, *e.g.*  $\text{Zn}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cd}^{2+}$  and  $\text{Ni}^{2+}$ . As an extension of work on the synthesis of oxadiazoles, we report here the crystal structure of (I) (Fig. 1), a new amidoxime which is the *Z* (*cis*) isomer. In the crystal structure, the molecules are linked through weak  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds, forming a dimeric structure (Fig. 2).



**Figure 1**

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

## Experimental

The reagents were purchased and used without further purification. 3-Chlorobenzohydroximinoyl chloride (6.01 g, 0.031 mol) was dissolved in dry  $\text{CHCl}_3$  (50 ml), then a solution of 1-naphthylamine (9.04 g, 0.0632 mol) in  $\text{CHCl}_3$  (10 ml) was added with stirring at room temperature. The reaction mixture was stirred for two days. The precipitate was filtered off and the excess solvent evaporated. The residue was subjected to flash column chromatography (hexane/ethyl acetate, 1:3), and allowed to evaporate slowly to give crystals.

### Crystal data

$\text{C}_{17}\text{H}_{13}\text{ClN}_2\text{O}$	$V = 747.41 (7) \text{ \AA}^3$
$M_r = 296.74$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.319 \text{ Mg m}^{-3}$
$a = 7.7217 (5) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.7039 (4) \text{ \AA}$	$\mu = 0.26 \text{ mm}^{-1}$
$c = 11.9158 (4) \text{ \AA}$	$T = 298 \text{ K}$
$\alpha = 104.099 (3)^\circ$	Block, orange
$\beta = 93.815 (4)^\circ$	$0.52 \times 0.30 \times 0.20 \text{ mm}$
$\gamma = 103.869 (4)^\circ$	

### Data collection

Bruker–Nonius KappaCCD diffractometer	2764 independent reflections
$\varphi$ and $\omega$ scans	1796 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.046$
10909 measured reflections	$\theta_{\text{max}} = 25.5^\circ$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 0.1831P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.110$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
2764 reflections	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
190 parameters	
H-atom parameters constrained	

**Table 1**

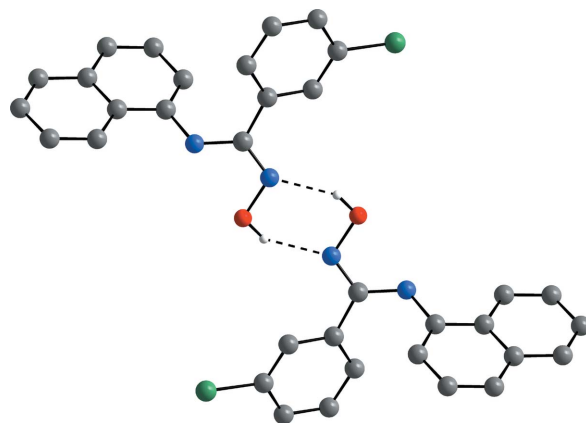
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1-H1O}\cdots\text{N1}^i$	0.88	1.98	2.768 (2)	147

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

All H atoms were located in a difference Fourier map. Aromatic H atoms were refined as riding on the respective C atoms with  $\text{C-H} = 0.93 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The O–H and N–H atoms were refined as riding in their as-found positions [ $\text{O-H} = 0.88 \text{ \AA}$ ,  $\text{N-H} = 0.95 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N,O})$ ].

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD*



**Figure 2**

The centrosymmetric dimer of (I). Hydrogen bonds are indicated by dashed lines. H atoms not involved in hydrogen bonds have been omitted.

(Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2006).

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## References

- Brandenburg, K. (2006). *DIAMOND*. Release 3.1d. Crystal Impact GbR, Bonn, Germany.
- Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
- Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
- Dürst, Y. (1998). *Magn. Reson. Chem.* **36**, 878–880.
- Kondo, K., Matsumoto, M. & Okamoto, K. (1999). *J. Chem. Eng. Jpn.* **32**, 217–222.
- Nieves-Neira, W., Rivera, M. I., Kohlhagen, G., Hursey, M. L., Pourquier, P., Sausville, E. A. & Pommie, Y. (1999). *Mol. Pharmacol.* **56**, 478–484.
- Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Seko, N., Tamada, M. & Yoshii, F. (2005). *Nucl. Instrum. Methods Phys. Res. B*, **236**, 21–29.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Westrip, S. (2006). *publCIF*. In preparation.
- Yu, J., Zhang, S., Li, Z., Lu, W. & Cai, M. (2005). *Bioorg. Med. Chem.* **13**, 353–361.
- Zhang, A., Uchiyama, G. & Asakura, T. (2005). *React. Funct. Polym.* **63**, 143–153.
- Zohuriaan-Mehr, M. J., Pourjavadi, A. & Salehi-Rad, M. (2004). *React. Funct. Polym.* **61**, 21–23.