

1,4-Bis(imidazol-1-ylmethyl)naphthalene

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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.044
 wR factor = 0.108
Data-to-parameter ratio = 9.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.In the title compound, $\text{C}_{18}\text{H}_{16}\text{N}_4$, the two imidazole rings are twisted away from the central naphthalene ring system by $81.4(1)$ and $88.4(1)^\circ$. The crystal packing is stabilized by $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds

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Comment

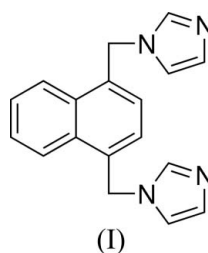
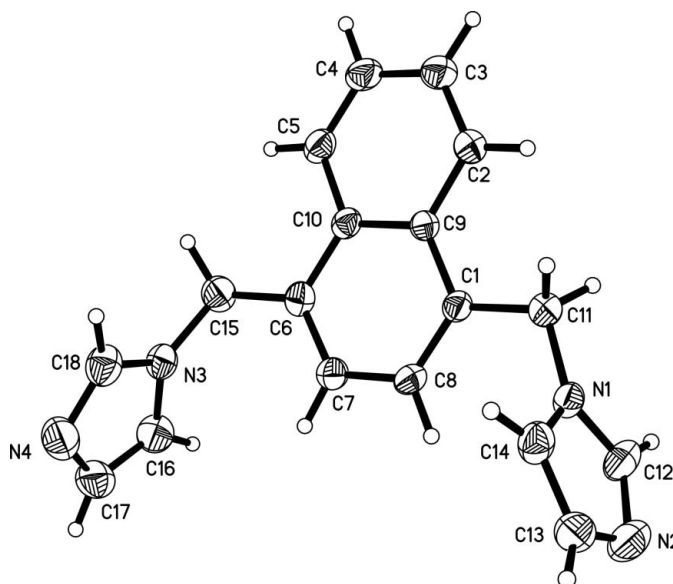
Numerous flexible or rigid *N*-heterocyclic carbene precursors have been synthesized and studied. They attract considerable attention because of their diverse coordination capabilities and the important catalytic properties of their metal complexes (Herrmann, 2002; Herrmann & Kocher, 1997). We report here the crystal structure of the title compound, (I).Bond lengths and angles in (I) are normal (Table 1). The naphthalene ring system is planar, with a maximum deviation of $0.048(2)$ Å for atom C6. The dihedral angle between the two imidazole rings is $43.7(1)^\circ$, and they are bound to the

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

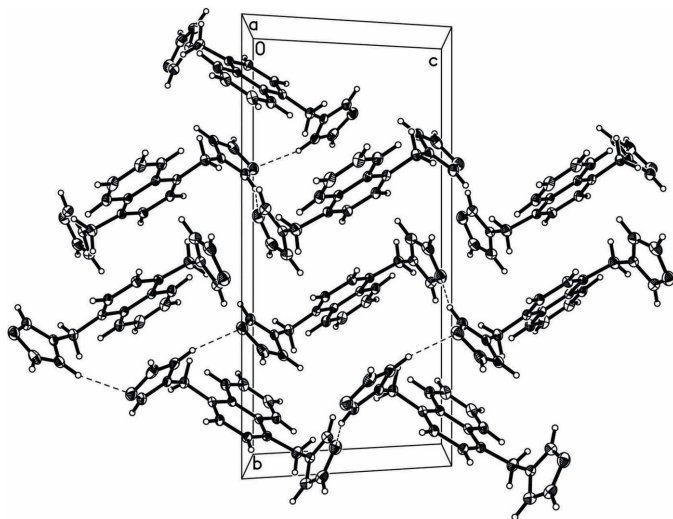


Figure 2

The crystal packing of (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

naphthalene ring system in a *cis* arrangement (Fig. 1). The N1/N2/C12–C14 and N3/N4/C16–C18 imidazole rings form dihedral angles of 81.4 (1) and 88.4 (1)°, respectively, with the naphthalene ring system. The crystal packing is stabilized by C–H···N hydrogen bonds (Fig. 2).

Experimental

Compound (I) was prepared according to the reported procedure of Dhal & Arnold (1992). Colourless single crystals suitable for X-ray diffraction were obtained by diffusion of diethyl ether vapour into a methanol solution.

Crystal data

$C_{18}H_{16}N_4$	$D_x = 1.314 \text{ Mg m}^{-3}$
$M_r = 288.35$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 20 reflections
$a = 8.222$ (4) Å	$\theta = 4.5\text{--}7.4^\circ$
$b = 19.541$ (8) Å	$\mu = 0.08 \text{ mm}^{-1}$
$c = 9.956$ (3) Å	$T = 293$ (2) K
$\beta = 114.31$ (3)°	Block, colourless
$V = 1457.8$ (10) Å ³	$0.28 \times 0.22 \times 0.18 \text{ mm}$
$Z = 4$	

Data collection

Enraf–Nonius CAD-4 diffractometer	$\theta_{\text{max}} = 25.0^\circ$
$\omega/2\theta$ scans	$h = -9 \rightarrow 8$
Absorption correction: none	$k = 0 \rightarrow 23$
2664 measured reflections	$l = 0 \rightarrow 11$
2568 independent reflections	3 standard reflections
1157 reflections with $I > 2\sigma(I)$	every 300 reflections
$R_{\text{int}} = 0.047$	intensity decay: none

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2]$
$wR(F^2) = 0.108$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.92$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2568 reflections	$\Delta\rho_{\text{max}} = 0.14 \text{ e \AA}^{-3}$
263 parameters	$\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (Å).

N1–C12	1.345 (3)	N3–C16	1.366 (4)
N1–C14	1.362 (3)	N3–C15	1.461 (3)
N1–C11	1.457 (3)	N4–C18	1.312 (4)
N2–C12	1.307 (4)	N4–C17	1.358 (4)
N2–C13	1.365 (4)	C4–C5	1.357 (4)
N3–C18	1.337 (3)	C5–C10	1.420 (3)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8–H8···N1	0.95 (2)	2.48 (2)	2.828 (4)	102 (2)
C12–H12···N4 ⁱ	1.01 (3)	2.55 (3)	3.465 (5)	152 (2)
C14–H14···N2 ⁱⁱ	0.95 (3)	2.53 (3)	3.416 (4)	155 (3)

Symmetry codes: (i) $x - 1, y, z - 1$; (ii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$.

H atoms were located in a difference Fourier map and refined isotropically. The range of C–H bond lengths is 0.88 (3)–1.03 (3) Å.

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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References

- Dhal, P. K. & Arnold, F. H. (1992). *Macromolecules*, **25**, 7051–7059.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
- Gabe, E. J. & White, P. S. (1993). *DIFRAC*. American Crystallographic Association, Pittsburgh Meeting, Abstract PA104.
- Herrmann, W. A. (2002). *Angew. Chem. Int. Ed.* **41**, 1290–1309.
- Herrmann, W. A. & Kocher, C. (1997). *Angew. Chem. Int. Ed. Engl.* **36**, 2162–2187.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.