Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

4-(2-Naphthyl)pyrimidine

Truls Ingebrigtsen, Tore Lejon and Lars Kr. Hansen*

Department of Chemistry, University of Tromsø, 9037 Tromsø, Norway

Correspondence e-mail: larsk@chem.uit.no

Received 6 June 2005
Accepted 17 June 2005
Online 24 June 2005

Key indicators

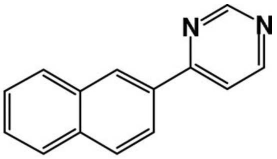
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.097
Data-to-parameter ratio = 9.8

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

The title compound, $C_{14}H_{10}N_2$, has been synthesized from the appropriate ketones and formamide using different palladium complexes as catalysts. The pyrimidine group is twisted 30.48 (9)° relative to the naphthalene part of the molecule, resulting in an intramolecular C—H···N hydrogen bond. There is also an intermolecular C—H···N hydrogen bond linking the molecules in the crystal structure.

Comment

Pyrimidines are widely found in nature, *e.g.* in pyrimidine and purine bases in nucleic acids, and in the vitamin thiamin. They have also attracted interest as potential drugs, and are available in the nucleoside analogue AZT^{TM} used in AIDS therapy, Acyclovir^{TM} used in treatment of herpes infections and in the prodrug Capecitabine^{TM} used in cancer therapy. The interesting chemical and physiological properties of pyrimidines have led to a number of syntheses being developed (von Angerer *et al.*, 2004). In our procedure, good yields of the expected products are formed from the appropriate ketone when reacted with formamide, catalysed by different palladium complexes (Ingebrigtsen *et al.*, 2005).



(I)

The atomic numbering scheme of the title compound, (I), is shown in Fig. 1. Bond lengths are within the normal range of such bonds (Allen *et al.*, 1987). The least-squares plane through the pyrimidine part of the molecule forms a dihedral angle of 30.48 (9)° with the naphthalene residue. This configuration allows for a short intramolecular hydrogen bond (C14—H14···N2). There is also a short intermolecular hydrogen bond (C1—H1···N1) contributing to the packing of the molecules in the crystal structure (Taylor & Kennard, 1982). Table 1 lists selected hydrogen bonds shorter than the van der Waals distance (Bondi, 1964).

Experimental

To a 10 ml flask charged with $Pd(OAc)_2$ (0.05 equivalents) and PPh_3 (0.10 equivalents) were added formamide (5.0 g), PhI (2.0 g) and ketone (1.0 equivalents). The resulting mixture was heated at 433 K for 8 h. The reaction mixture was diluted with diethyl ether and extracted three times with 2 *M* HCl. The combined aqueous layers were basified with 4 *M* NaOH and extracted with diethyl ether. The organic layer was washed with water and brine and dried over Na_2CO_3. Evaporation of the solvent gave the crude product as a white solid. Purification by silica column chromatography (EtOAc), gave crystals that were dissolved in a small amount of diethyl ether. Heptane was added and crystals of the title compound were grown by slow evaporation of the solvent at room temperature.

Crystal data

$C_{14}H_{10}N_2$
$M_r = 206.24$
Monoclinic, $P2_1/a$
$a = 7.4467$ (16) Å
$b = 6.1343$ (11) Å
$c = 22.720$ (3) Å
$\beta = 92.508$ (19)°
$V = 1036.9$ (3) Å^3
$Z = 4$

$D_x = 1.321$ Mg m$^{-3$}
Mo *Kα* radiation
Cell parameters from 25 reflections
$\theta = 12$–18°
$\mu = 0.08$ mm^{-1}
$T = 298$ (2) K
Plate, white
0.50 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan [North *et al.*, (1968) and *ABSCALC* in *OSCAIL* (McArdle & Daly, 1999)]
$T_{\min} = 0.961$, $T_{\max} = 0.992$
1984 measured reflections
1813 independent reflections

586 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.008$
$\theta_{\max} = 24.9°$
$h = -2 \rightarrow 8$
$k = 0 \rightarrow 7$
$l = -26 \rightarrow 26$
3 standard reflections frequency: 120 min intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.097$
$S = 0.82$
1813 reflections
185 parameters

All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.035$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···N2	1.01 (2)	2.49 (3)	2.827 (4)	99 (2)
C1—H1···N1$^{\rm i}$	0.93 (2)	2.60 (3)	3.440 (5)	151 (2)
C13—H13···C6$^{\rm ii}$	1.00 (2)	2.78 (3)	3.735 (5)	163 (2)
C8—H8···C11$^{\rm iii}$	0.98 (2)	2.82 (3)	3.716 (3)	153 (2)

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

All the H atoms were found in a difference map and were refined independently; C—H = 0.93 (3)–1.07 (3) Å. The quality of the crystal was rather poor and accordingly data were collected only to $\theta_{\max}$ = 24.9°.

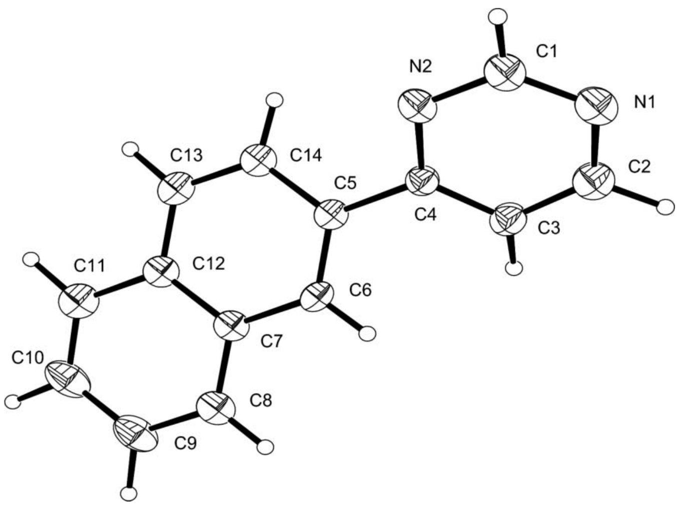


Figure 1
A view of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1992); cell refinement: *CELDIM* in *CAD-4-PC Software*; data reduction: *XCAD4* (McArdle & Higgins, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *OSCAIL* (McArdle, 1993).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Angerer, S. von (2004). *Methods Synth.* **16**, 379–572.
Bondi, A. (1964). *J. Chem. Phys.* **68**, 441–451.
Enraf–Nonius (1992). *CAD-4-PC Software*. Version 1.1. Enraf–Nonius, Delft, The Netherlands.
Ingebrigtsen, T., Helland, I. & Lejon, T. (2005). *Heterocycles.* Submitted.
McArdle, P. (1993). *J. Appl. Cryst.* **26**, 752.
McArdle, P. (1995). *J. Appl. Cryst.* **28**, 65.
McArdle, P. & Daly, P. (1999). *ABSCALC.* PC version. National University of Ireland, Galway, Ireland.
McArdle, P. & Higgins, T. (1995). *XCAD4*. National University of Ireland, Galway, Ireland.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Taylor, R. & Kennard, O. (1982). *J. Am. Chem. Soc.* **104**, 5063–5070.

Acta Cryst. (2005). E**61**, o2256–o2257 Ingebrigtsen *et al.* • $C_{14}H_{10}N_2$ **o2257**