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N-Acetyl-*N*-[1-(2-naphthalenyl)ethenyl]acetamide

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The crystal structure of the title compound, $C_{16}H_{15}NO_2$, is stabilized by weak intermolecular C—H···O hydrogen bonds and C—H···π interactions.

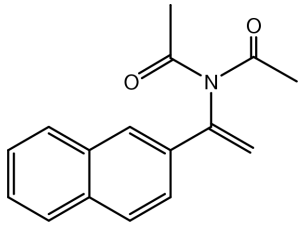
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.164
Data-to-parameter ratio = 18.2

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

Comment

The title compound, *N*-acetyl-*N*-[1-(2-naphthalenyl)ethenyl]-acetamide, (I), was obtained as a by-product when we synthesized *N*-[1-(2-naphthalenyl)ethenyl]acetamide (Burk *et al.*, 1998). In (I), the dihedral angle between the planar naphthalene moiety and the plane consisting of N1, O1, O2, C13–C16 is 82.76 (5)°. The crystal structure is stabilized by C—H···O and C—H···π interactions (Table 1). In Table 1, $Cg(A)$ and $Cg(B)$ denote the centres of gravity of the two phenyl rings C3–C6, C11, C12 and C6–C11, respectively.



(I)

Experimental

Acetic anhydride (8.39 g, 82.3 mmol), followed by acetic acid (4.94 g, 82.3 mmol), was added to a solution of 2-acetonaphthone oxime (5.07 g, 27.4 mmol) in toluene (40 ml) under a nitrogen atmosphere. Fe powder (3.08 g, 55 mmol) was then added and the mixture was heated to 353 K for 48 h. The reaction was then cooled to room temperature and filtered through celite to remove solid residues, which were then washed with toluene (2 × 5 ml). The combined filtrates were diluted with ethyl acetate (50 ml) and the mixture cooled in an ice bath and washed with 2 M NaOH (2 × 30 ml). The organic phase was separated, dried over Na_2SO_4, and the solvents were evaporated. The solid was separated and purified by column chromatography with dichloromethane as eluent. The desired product was recrystallized from chloroform. 1H NMR δ (*p.p*,m.): 7.26–7.86 (*m*, 7H), 6.17 (*s*, 1H), 5.42 (*s*, 1H), 2.46 (*s*, 6H).

Crystal data

$C_{16}H_{15}NO_2$
M_r = 253.29
Orthorhombic, *Pbca*
a = 8.9909 (17) Å
b = 14.814 (3) Å
c = 20.469 (4) Å
V = 2726.3 (9) Å^3
Z = 8
D_x = 1.234 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2575 reflections
θ = 1–27.5°
μ = 0.08 mm^{-1}
T = 294 (2) K
Block, colorless
0.30 × 0.24 × 0.22 mm

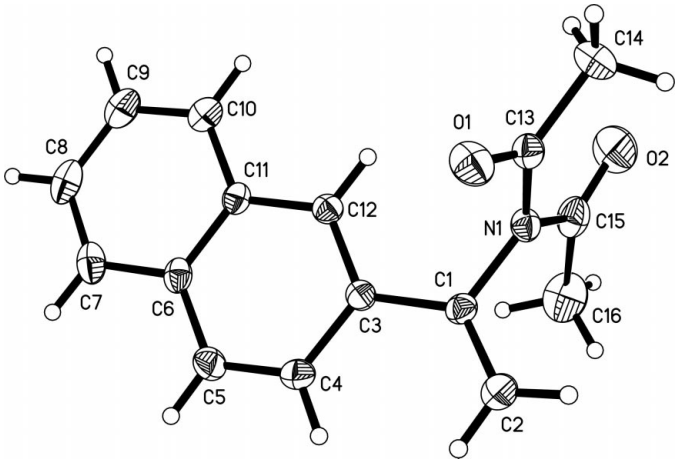


Figure 1
The molecular structure of (I). Displacement ellipsoids are shown at the 30% probability level.

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.982
17598 measured reflections

3163 independent reflections
994 reflections with $I > 2\sigma(I)$
R_{int} = 0.102
θ_{max} = 27.7°
$h = -10 \rightarrow 11$
$k = -19 \rightarrow 19$
$l = -25 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.164
S = 0.96
3172 reflections
174 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···O1^{i}	0.93	2.57	3.312 (4)	137
C5—H5···O1^{ii}	0.93	2.51	3.370 (4)	154
C2—H2B···Cg(A^{i})	0.93	2.96	3.578 (3)	125
C4—H4···Cg(B^{i})	0.93	3.15	3.999 (3)	154
C14—H14C···Cg(A^{iii})	0.96	3.03	3.728 (4)	131

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

The H atoms were placed in their geometrically calculated positions and included in the final refinement in the riding model approximation. Owing to the poor diffraction quality of the crystal, the ratio of observed to unique reflections is low (31%) and the R_{int} value is high (0.102).

Data collection: *SMART* (Bruker, 1995); cell refinement: *SMART*; data reduction: *SHELXTL* (Bruker, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Burk, M. J., Casy, G. & Johnson, N. B. (1998). *J. Org. Chem.* **63**, 6084–6085.
Bruker (1995). *SMART* (Version 5.0) and *SHELXTL-NT* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.