(*E*)-1-(2-Nitroethenyl)naphthalene

Lin-Hai Jing

School of Chemistry and Chemical Engineering, China West Normal University, Nanchong 637002, People's Republic of China

Correspondence e-mail: jlhjhr@yahoo.com.cn

The title molecule, $C_{12}H_9NO_2$, adopts a *trans* configuration about the olefinic double bond. The dihedral angle between the naphthalene ring system (r.m.s. deviation = 0.012 Å) and the nitroethenyl group (r.m.s. deviation = 0.032 Å) is 12.66 (5)°. The molecules are linked into a two-dimensional network parallel to the *bc* plane by C—H⋯O hydrogen bonds. The substituted benzene rings in adjacent networks are stacked with a centroid–centroid distance of 3.6337 (11) Å, indicating π–π interactions.

Related literature

For general background to β-nitroolefins, see: Barrett & Graboski (1986). For the synthesis, see: Cheng *et al.* (2007).
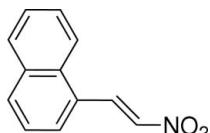
Experimental

Crystal data

$C_{12}H_9NO_2$

$M_r = 199.20$

Orthorhombic, *Pbca*

$a = 7.2670\ (14)$ Å

$b = 13.741\ (3)$ Å

$c = 19.127\ (4)$ Å

$V = 1909.9\ (6)$ Å^3

$Z = 8$

Mo $K\alpha$ radiation

$\mu = 0.10$ mm^{-1}

$T = 93$ K

$0.40 \times 0.33 \times 0.13$ mm

Data collection

Rigaku SPIDER diffractometer

Absorption correction: none

14290 measured reflections

2179 independent reflections

2019 reflections with $I > 2\sigma(I)$

$R_{int} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.099$

$S = 1.00$

2179 reflections

136 parameters

H-atom parameters constrained

$\Delta\rho_{max} = 0.30$ e Å^{-3}

$\Delta\rho_{min} = -0.20$ e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C2—H2⋯O2[i]	0.95	2.58	3.3919 (19)	144
C7—H7⋯O2[ii]	0.95	2.52	3.4261 (19)	159
C12—H12⋯O2[i]	0.95	2.57	3.464 (2)	158

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

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2915).

References

Barrett, A. G. M. & Graboski, G. G. (1986). *Chem. Rev.* **86**, 751–762.

Cheng, P., Jiang, Z. Y., Wang, R. R., Zhang, X. M., Wang, Q., Zheng, Y. T., Zhou, J. & Chen, J. J. (2007). *Bioorg. Med. Chem. Lett.* **17**, 4476–4480.

Rigaku/MSC (2004). *RAPID-AUTO*. Rigaku/MSC Inc., The Woodlands, Texas, USA.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

(*E*)-1-(2-Nitroethenyl)naphthalene

L.-H. Jing

Comment

β-Nitroolefins are a class of useful and versatile building blocks in organic synthesis (Barrett & Graboski, 1986). The author reports here, the crystal structure of the title compound.

Bond lengths and angles in the title molecule are normal. The molecule adopts a trans configuration about the olefinic double bond (Fig. 1). The naphthalene ring system is planar, with a maximum deviation of 0.021 (1) Å for atom C1. The dihedral angle between the C1-C9 and N1/O1/O2/C11/C12 planes is 12.66 (5)°. The molecules are linked into a two-dimensional network parallel to the *bc* plane by C—H···O hydrogen bonds (Table 1).

Experimental

The title compound was synthesized according to the method reported in the literature (Cheng *et al.*, 2007). Yellow single crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution.

Refinement

All H atoms were placed in calculated positions, with C-H = 0.95 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures
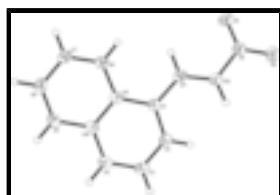
Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering.

(*E*)-1-(2-Nitroethenyl)naphthalene

Crystal data

$C_{12}H_9NO_2$	$F_{000} = 832$
$M_r = 199.20$	$D_x = 1.386$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 5654 reflections
$a = 7.2670$ (14) Å	θ = 3.0–27.5°
$b = 13.741$ (3) Å	μ = 0.10 mm^{-1}

$c = 19.127\ (4)$ Å

$V = 1909.9\ (6)$ Å^3

$Z = 8$

$T = 93$ K

Prism, yellow

$0.40 \times 0.33 \times 0.13$ mm

Data collection

Rigaku SPIDER diffractometer	2019 reflections with $I > 2\sigma(I)$
Radiation source: Rotating anode	$R_{int} = 0.030$
Monochromator: graphite	$\theta_{max} = 27.5°$
$T = 93$ K	$\theta_{min} = 3.2°$
ω scans	$h = -9 \rightarrow 9$
Absorption correction: none	$k = -17 \rightarrow 17$
14290 measured reflections	$l = -24 \rightarrow 24$
2179 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.099$	$w = 1/[\sigma^2(F_o^2) + (0.0285P)^2 + 1.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
2179 reflections	$\Delta\rho_{max} = 0.30$ e Å^{-3}
136 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
O1	0.4804 (2)	0.25001 (8)	0.56207 (6)	0.0438 (4)
O2	0.4755 (2)	0.35241 (8)	0.47651 (6)	0.0414 (3)
N1	0.50070 (19)	0.33185 (9)	0.53854 (6)	0.0270 (3)

C1	0.61925 (19)	0.47388 (10)	0.70231 (7)	0.0193 (3)
C2	0.67974 (19)	0.56401 (10)	0.67959 (8)	0.0216 (3)
H2	0.6907	0.5759	0.6308	0.026*
C3	0.7251 (2)	0.63794 (10)	0.72673 (8)	0.0233 (3)
H3	0.7665	0.6991	0.7097	0.028*
C4	0.7103 (2)	0.62294 (10)	0.79730 (8)	0.0237 (3)
H4	0.7403	0.6740	0.8288	0.028*
C5	0.6346 (2)	0.51571 (11)	0.89674 (8)	0.0250 (3)
H5	0.6628	0.5669	0.9283	0.030*
C6	0.5794 (2)	0.42761 (11)	0.92232 (8)	0.0260 (3)
H6	0.5693	0.4178	0.9713	0.031*
C7	0.5373 (2)	0.35112 (11)	0.87574 (8)	0.0246 (3)
H7	0.5001	0.2897	0.8936	0.030*
C8	0.5497 (2)	0.36480 (10)	0.80489 (7)	0.0216 (3)
H8	0.5198	0.3126	0.7744	0.026*
C9	0.60624 (18)	0.45543 (9)	0.77616 (7)	0.0189 (3)
C10	0.65057 (19)	0.53203 (10)	0.82360 (8)	0.0204 (3)
C11	0.5682 (2)	0.39854 (10)	0.65200 (7)	0.0219 (3)
H11	0.5419	0.3356	0.6700	0.026*
C12	0.5554 (2)	0.41047 (11)	0.58392 (8)	0.0278 (3)
H12	0.5829	0.4723	0.5642	0.033*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0825 (10)	0.0188 (5)	0.0300 (6)	−0.0081 (6)	0.0015 (6)	−0.0001 (5)
O2	0.0744 (10)	0.0281 (6)	0.0216 (6)	−0.0004 (6)	−0.0060 (6)	−0.0006 (5)
N1	0.0370 (7)	0.0208 (6)	0.0231 (6)	0.0009 (6)	0.0016 (5)	−0.0004 (5)
C1	0.0165 (6)	0.0179 (6)	0.0236 (7)	0.0030 (5)	−0.0002 (5)	0.0002 (5)
C2	0.0190 (7)	0.0218 (7)	0.0241 (7)	0.0022 (5)	−0.0003 (5)	0.0033 (6)
C3	0.0191 (7)	0.0169 (6)	0.0339 (8)	−0.0018 (5)	−0.0003 (6)	0.0030 (6)
C4	0.0209 (7)	0.0195 (6)	0.0306 (8)	0.0003 (5)	−0.0013 (6)	−0.0041 (6)
C5	0.0242 (7)	0.0255 (7)	0.0252 (7)	0.0034 (6)	−0.0003 (6)	−0.0054 (6)
C6	0.0281 (8)	0.0285 (7)	0.0214 (7)	0.0056 (6)	0.0031 (6)	0.0010 (6)
C7	0.0259 (7)	0.0209 (7)	0.0270 (7)	0.0040 (6)	0.0052 (6)	0.0048 (6)
C8	0.0223 (7)	0.0174 (6)	0.0250 (7)	0.0030 (5)	0.0011 (6)	−0.0002 (5)
C9	0.0147 (6)	0.0175 (6)	0.0245 (7)	0.0038 (5)	0.0009 (5)	−0.0001 (5)
C10	0.0157 (6)	0.0200 (7)	0.0255 (7)	0.0030 (5)	−0.0002 (5)	−0.0014 (5)
C11	0.0242 (7)	0.0167 (6)	0.0249 (7)	0.0021 (5)	0.0003 (6)	0.0016 (5)
C12	0.0389 (9)	0.0185 (7)	0.0260 (7)	−0.0042 (6)	−0.0012 (7)	−0.0003 (6)

Geometric parameters (Å, °)

O1—N1	1.2201 (17)	C5—C10	1.422 (2)
O2—N1	1.2335 (16)	C5—H5	0.95
N1—C12	1.4417 (19)	C6—C7	1.411 (2)
C1—C2	1.3841 (19)	C6—H6	0.95
C1—C9	1.4381 (19)	C7—C8	1.371 (2)
C1—C11	1.4613 (19)	C7—H7	0.95

C2—C3	1.398 (2)	C8—C9	1.4220 (19)
C2—H2	0.95	C8—H8	0.95
C3—C4	1.370 (2)	C9—C10	1.4265 (19)
C3—H3	0.95	C11—C12	1.316 (2)
C4—C10	1.415 (2)	C11—H11	0.95
C4—H4	0.95	C12—H12	0.95
C5—C6	1.366 (2)		
O1—N1—O2	123.23 (13)	C7—C6—H6	120.1
O1—N1—C12	120.13 (13)	C8—C7—C6	120.51 (14)
O2—N1—C12	116.64 (12)	C8—C7—H7	119.7
C2—C1—C9	119.15 (13)	C6—C7—H7	119.7
C2—C1—C11	120.51 (13)	C7—C8—C9	121.40 (13)
C9—C1—C11	120.34 (12)	C7—C8—H8	119.3
C1—C2—C3	121.50 (13)	C9—C8—H8	119.3
C1—C2—H2	119.3	C8—C9—C10	117.75 (13)
C3—C2—H2	119.3	C8—C9—C1	123.58 (13)
C4—C3—C2	120.52 (13)	C10—C9—C1	118.67 (13)
C4—C3—H3	119.7	C4—C10—C5	120.94 (13)
C2—C3—H3	119.7	C4—C10—C9	119.65 (13)
C3—C4—C10	120.48 (13)	C5—C10—C9	119.42 (13)
C3—C4—H4	119.8	C12—C11—C1	125.55 (13)
C10—C4—H4	119.8	C12—C11—H11	117.2
C6—C5—C10	121.07 (14)	C1—C11—H11	117.2
C6—C5—H5	119.5	C11—C12—N1	121.46 (14)
C10—C5—H5	119.5	C11—C12—H12	119.3
C5—C6—C7	119.84 (14)	N1—C12—H12	119.3
C5—C6—H6	120.1		
C9—C1—C2—C3	−1.2 (2)	C3—C4—C10—C5	−179.96 (14)
C11—C1—C2—C3	178.42 (13)	C3—C4—C10—C9	0.2 (2)
C1—C2—C3—C4	−0.1 (2)	C6—C5—C10—C4	−179.12 (14)
C2—C3—C4—C10	0.6 (2)	C6—C5—C10—C9	0.7 (2)
C10—C5—C6—C7	0.0 (2)	C8—C9—C10—C4	179.02 (12)
C5—C6—C7—C8	−0.7 (2)	C1—C9—C10—C4	−1.6 (2)
C6—C7—C8—C9	0.5 (2)	C8—C9—C10—C5	−0.79 (19)
C7—C8—C9—C10	0.2 (2)	C1—C9—C10—C5	178.64 (13)
C7—C8—C9—C1	−179.20 (14)	C2—C1—C11—C12	−7.4 (2)
C2—C1—C9—C8	−178.57 (13)	C9—C1—C11—C12	172.20 (15)
C11—C1—C9—C8	1.8 (2)	C1—C11—C12—N1	−178.90 (14)
C2—C1—C9—C10	2.03 (19)	O1—N1—C12—C11	−6.4 (2)
C11—C1—C9—C10	−177.61 (12)	O2—N1—C12—C11	173.19 (16)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O2[i]	0.95	2.58	3.3919 (19)	144
C7—H7···O2[ii]	0.95	2.52	3.4261 (19)	159
C12—H12···O2[i]	0.95	2.57	3.464 (2)	158

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, −*y*+1/2, *z*+1/2.

Fig. 1