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N-[3-(2-Nitrophenyl)allylidene]-naphthalen-1-amine

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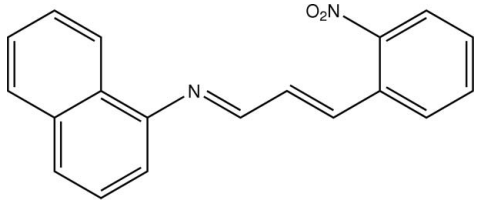
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.124; data-to-parameter ratio = 14.0.

In the crystal structure of the title compound, $C_{19}H_{14}N_2O_2$, the molecules are almost planar. The dihedral angle between the two aromatic ring systems is 3.67 (1)°.

Related literature

For related literature, see: Yang *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{14}N_2O_2$
M_r = 302.32
Monoclinic, $P2_1/c$
a = 15.440 (2) Å
b = 7.4165 (10) Å
c = 14.598 (2) Å
β = 117.347 (2)°
V = 1484.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.42 × 0.26 × 0.05 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.996
8073 measured reflections
2913 independent reflections
2014 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.124
S = 1.02
2913 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1997), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2032).

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Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
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supplementary materials

Acta Cryst. (2007). E**63**, o2919 [**doi:10.1107/S1600536807022453**]

N-[3-(2-Nitrophenyl)allylidene]naphthalen-1-amine

X.-Y. Yang, X.-L. He, Y. Li and S. Bi

Comment

As part of our ongoing studies on push-pull Schiff bases, the title compound was synthesized and its crystal structure was determined (Yang *et al.*, 2006).

The molecule is almost planar with a dihedral angle of 3.67 (1)° between the two aromatic rings (Fig. 1). As expected, the bond lengths between the benzene and naphthalene rings in (I) alternates. In the crystal structure the molecules are stacked onto each other with distances of 3.782 and 3.731 Å between the centroids of the rings, indicating for π-π interactions.

Experimental

Compound (I) was prepared according to the method of Yang *et al.* (2006). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of the solvent from an ethanol-water (4:1 *v*/*v*) solution over a period of 3 d.

Refinement

The H atoms were positioned with idealized geometry and were refined isotropic with U_{iso}(H) = 1.2 U_{eq}(C) using a riding model with C—H distances of 0.93 Å.

Figures

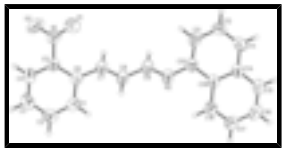


Fig. 1. Crystal structure of I showing 50% probability displacement ellipsoids and the atom numbering scheme.

N-[3-(2-Nitrophenyl)allylidene]naphthalen-1-amine

Crystal data

$C_{19}H_{14}N_2O_2$	F_{000} = 632
M_r = 302.32	D_x = 1.352 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 15.440 (2) Å	Cell parameters from 1605 reflections
b = 7.4165 (10) Å	θ = 2.8–23.8º
c = 14.598 (2) Å	μ = 0.09 mm^{-1}
β = 117.347 (2)º	T = 293 (2) K
V = 1484.7 (3) Å^3	Plate, yellow

$Z = 4$	0.42 × 0.26 × 0.05 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2913 independent reflections
Radiation source: fine-focus sealed tube	2014 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.039$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.1°$
$T = 293(2)$ K	$\theta_{min} = 1.5°$
ω scans	$h = -19\rightarrow12$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -9\rightarrow8$
$T_{min} = 0.964$, $T_{max} = 0.996$	$l = -18\rightarrow17$
8073 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.124$	$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.0855P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
2913 reflections	$\Delta\rho_{max} = 0.13$ e Å^{-3}
208 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 $F^2 > 2\text{sigma}(F^2)$ 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}
C19	0.18422 (11)	0.8023 (2)	0.42612 (12)	0.0389 (4)
C6	−0.25313 (11)	0.6242 (2)	0.47210 (13)	0.0413 (4)
N2	0.02462 (10)	0.7772 (2)	0.41815 (11)	0.0487 (4)

N1	−0.40204 (11)	0.5240 (2)	0.31629 (12)	0.0548 (4)
C5	−0.35316 (11)	0.5882 (2)	0.42333 (12)	0.0420 (4)
C10	0.08469 (11)	0.7471 (2)	0.37018 (13)	0.0417 (4)
C1	−0.21576 (13)	0.6856 (2)	0.57357 (14)	0.0504 (5)
H1A	−0.1493	0.7096	0.6101	0.061*
C7	−0.18684 (11)	0.5971 (2)	0.42695 (13)	0.0466 (4)
H7A	−0.1989	0.5005	0.3821	0.056*
C11	0.05107 (13)	0.6791 (2)	0.27212 (14)	0.0519 (5)
H11A	−0.0135	0.6421	0.2361	0.062*
C14	0.24596 (11)	0.7850 (2)	0.37904 (13)	0.0424 (4)
C4	−0.41129 (13)	0.6127 (2)	0.47087 (15)	0.0518 (5)
H4A	−0.4775	0.5865	0.4358	0.062*
C13	0.20743 (13)	0.7164 (3)	0.27765 (14)	0.0523 (5)
H13A	0.2475	0.7066	0.2459	0.063*
C9	−0.04464 (12)	0.6684 (2)	0.40303 (14)	0.0494 (5)
H9A	−0.0528	0.5655	0.3635	0.059*
C12	0.11219 (13)	0.6645 (3)	0.22567 (14)	0.0553 (5)
H12A	0.0879	0.6192	0.1590	0.066*
C18	0.22384 (12)	0.8694 (2)	0.52798 (13)	0.0458 (4)
H18A	0.1839	0.8819	0.5596	0.055*
C17	0.31968 (13)	0.9160 (2)	0.58045 (14)	0.0525 (5)
H17A	0.3446	0.9597	0.6475	0.063*
C2	−0.27333 (15)	0.7122 (3)	0.62153 (15)	0.0582 (5)
H2B	−0.2458	0.7547	0.6890	0.070*
C15	0.34514 (12)	0.8360 (2)	0.43613 (15)	0.0509 (5)
H15A	0.3865	0.8264	0.4059	0.061*
C16	0.38070 (13)	0.8985 (2)	0.53407 (15)	0.0553 (5)
H16A	0.4462	0.9299	0.5706	0.066*
O2	−0.47769 (10)	0.4391 (2)	0.28762 (11)	0.0802 (5)
O1	−0.36607 (10)	0.5584 (3)	0.25959 (10)	0.0848 (5)
C8	−0.11034 (12)	0.7017 (2)	0.44595 (14)	0.0493 (5)
H8A	−0.0989	0.8009	0.4890	0.059*
C3	−0.37129 (15)	0.6760 (3)	0.57018 (16)	0.0585 (5)
H3A	−0.4103	0.6943	0.6025	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C19	0.0397 (9)	0.0348 (9)	0.0434 (9)	0.0039 (7)	0.0203 (8)	0.0073 (7)
C6	0.0381 (9)	0.0376 (9)	0.0486 (10)	0.0023 (7)	0.0203 (8)	0.0062 (7)
N2	0.0363 (8)	0.0543 (9)	0.0576 (9)	0.0043 (7)	0.0233 (7)	0.0046 (7)
N1	0.0438 (9)	0.0663 (10)	0.0467 (9)	0.0024 (8)	0.0142 (8)	0.0057 (8)
C5	0.0391 (9)	0.0423 (9)	0.0437 (9)	0.0014 (7)	0.0183 (8)	0.0049 (8)
C10	0.0359 (9)	0.0431 (10)	0.0463 (10)	0.0052 (7)	0.0192 (8)	0.0074 (8)
C1	0.0442 (10)	0.0497 (11)	0.0519 (11)	−0.0041 (8)	0.0173 (9)	−0.0010 (8)
C7	0.0403 (10)	0.0476 (10)	0.0532 (10)	0.0030 (8)	0.0225 (8)	0.0034 (8)
C11	0.0397 (10)	0.0581 (11)	0.0484 (10)	−0.0003 (8)	0.0122 (8)	0.0065 (9)
C14	0.0409 (9)	0.0413 (10)	0.0469 (10)	0.0042 (7)	0.0218 (8)	0.0086 (8)

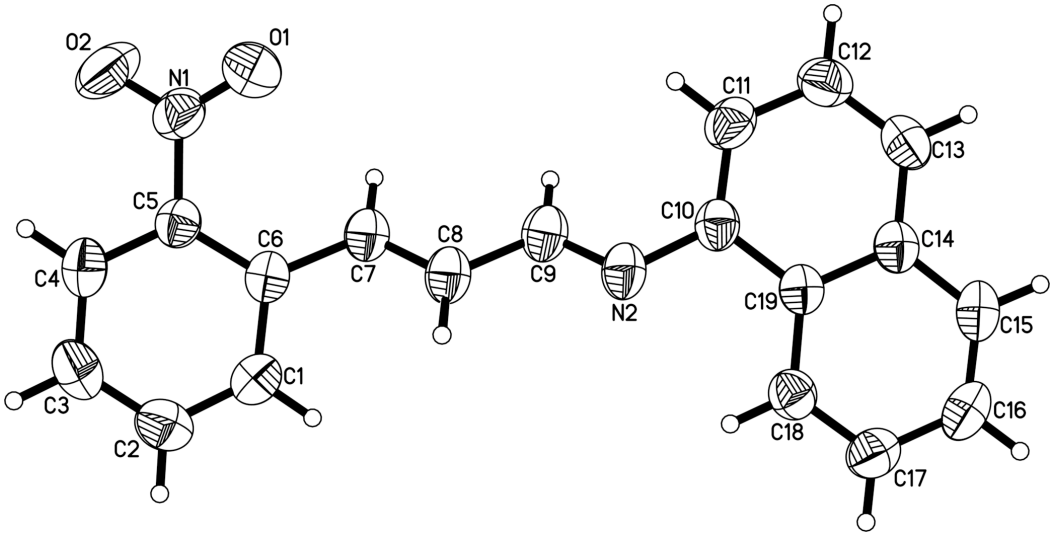
C4	0.0443 (10)	0.0515 (11)	0.0659 (12)	−0.0009 (8)	0.0306 (10)	0.0038 (9)
C13	0.0552 (11)	0.0605 (12)	0.0500 (11)	0.0076 (9)	0.0317 (9)	0.0065 (9)
C9	0.0381 (9)	0.0499 (11)	0.0596 (11)	0.0067 (8)	0.0218 (9)	0.0063 (9)
C12	0.0564 (12)	0.0661 (13)	0.0422 (10)	0.0027 (9)	0.0215 (9)	0.0013 (9)
C18	0.0492 (10)	0.0444 (10)	0.0471 (10)	−0.0002 (8)	0.0249 (9)	0.0023 (8)
C17	0.0521 (11)	0.0508 (11)	0.0471 (10)	−0.0059 (8)	0.0163 (9)	0.0005 (9)
C2	0.0704 (13)	0.0532 (12)	0.0553 (11)	−0.0028 (10)	0.0325 (10)	−0.0055 (9)
C15	0.0421 (10)	0.0518 (11)	0.0645 (12)	0.0020 (8)	0.0293 (9)	0.0115 (9)
C16	0.0394 (10)	0.0531 (11)	0.0640 (12)	−0.0076 (8)	0.0155 (9)	0.0065 (9)
O2	0.0538 (9)	0.1017 (12)	0.0619 (9)	−0.0247 (8)	0.0067 (7)	−0.0022 (8)
O1	0.0686 (10)	0.1381 (16)	0.0511 (8)	−0.0080 (9)	0.0304 (8)	−0.0017 (9)
C8	0.0392 (10)	0.0510 (11)	0.0589 (11)	0.0057 (8)	0.0235 (9)	0.0062 (9)
C3	0.0675 (13)	0.0547 (12)	0.0711 (13)	0.0005 (9)	0.0472 (11)	−0.0016 (10)

Geometric parameters (Å, °)

C19—C18	1.413 (2)	C14—C15	1.418 (2)
C19—C14	1.414 (2)	C4—C3	1.371 (3)
C19—C10	1.429 (2)	C4—H4A	0.9300
C6—C1	1.396 (2)	C13—C12	1.364 (2)
C6—C5	1.398 (2)	C13—H13A	0.9300
C6—C7	1.464 (2)	C9—C8	1.438 (2)
N2—C9	1.275 (2)	C9—H9A	0.9300
N2—C10	1.413 (2)	C12—H12A	0.9300
N1—O1	1.2171 (18)	C18—C17	1.362 (2)
N1—O2	1.2192 (18)	C18—H18A	0.9300
N1—C5	1.468 (2)	C17—C16	1.396 (2)
C5—C4	1.376 (2)	C17—H17A	0.9300
C10—C11	1.375 (2)	C2—C3	1.371 (3)
C1—C2	1.375 (2)	C2—H2B	0.9300
C1—H1A	0.9300	C15—C16	1.356 (3)
C7—C8	1.331 (2)	C15—H15A	0.9300
C7—H7A	0.9300	C16—H16A	0.9300
C11—C12	1.396 (2)	C8—H8A	0.9300
C11—H11A	0.9300	C3—H3A	0.9300
C14—C13	1.412 (2)		
C18—C19—C14	118.73 (15)	C12—C13—C14	120.81 (17)
C18—C19—C10	122.28 (15)	C12—C13—H13A	119.6
C14—C19—C10	118.96 (15)	C14—C13—H13A	119.6
C1—C6—C5	115.11 (15)	N2—C9—C8	121.30 (18)
C1—C6—C7	119.26 (15)	N2—C9—H9A	119.3
C5—C6—C7	125.60 (16)	C8—C9—H9A	119.3
C9—N2—C10	120.23 (16)	C13—C12—C11	120.28 (17)
O1—N1—O2	122.65 (17)	C13—C12—H12A	119.9
O1—N1—C5	118.92 (15)	C11—C12—H12A	119.9
O2—N1—C5	118.43 (16)	C17—C18—C19	120.97 (16)
C4—C5—C6	122.82 (16)	C17—C18—H18A	119.5
C4—C5—N1	116.38 (15)	C19—C18—H18A	119.5
C6—C5—N1	120.79 (15)	C18—C17—C16	120.30 (17)

C11—C10—N2	123.64 (15)	C18—C17—H17A	119.9
C11—C10—C19	119.50 (15)	C16—C17—H17A	119.9
N2—C10—C19	116.74 (15)	C3—C2—C1	120.16 (19)
C2—C1—C6	122.55 (17)	C3—C2—H2B	119.9
C2—C1—H1A	118.7	C1—C2—H2B	119.9
C6—C1—H1A	118.7	C16—C15—C14	121.05 (17)
C8—C7—C6	124.28 (17)	C16—C15—H15A	119.5
C8—C7—H7A	117.9	C14—C15—H15A	119.5
C6—C7—H7A	117.9	C15—C16—C17	120.43 (16)
C10—C11—C12	121.18 (16)	C15—C16—H16A	119.8
C10—C11—H11A	119.4	C17—C16—H16A	119.8
C12—C11—H11A	119.4	C7—C8—C9	123.05 (18)
C13—C14—C19	119.25 (15)	C7—C8—H8A	118.5
C13—C14—C15	122.24 (16)	C9—C8—H8A	118.5
C19—C14—C15	118.51 (16)	C2—C3—C4	119.54 (18)
C3—C4—C5	119.81 (17)	C2—C3—H3A	120.2
C3—C4—H4A	120.1	C4—C3—H3A	120.2
C5—C4—H4A	120.1		
C1—C6—C5—C4	0.6 (2)	C18—C19—C14—C15	−0.1 (2)
C7—C6—C5—C4	178.47 (15)	C10—C19—C14—C15	−178.49 (14)
C1—C6—C5—N1	179.58 (15)	C6—C5—C4—C3	0.4 (3)
C7—C6—C5—N1	−2.5 (3)	N1—C5—C4—C3	−178.66 (16)
O1—N1—C5—C4	154.51 (17)	C19—C14—C13—C12	−1.0 (3)
O2—N1—C5—C4	−25.0 (2)	C15—C14—C13—C12	178.42 (16)
O1—N1—C5—C6	−24.5 (2)	C10—N2—C9—C8	−176.27 (14)
O2—N1—C5—C6	155.98 (16)	C14—C13—C12—C11	0.2 (3)
C9—N2—C10—C11	36.7 (2)	C10—C11—C12—C13	0.6 (3)
C9—N2—C10—C19	−147.33 (16)	C14—C19—C18—C17	−0.3 (2)
C18—C19—C10—C11	−178.51 (16)	C10—C19—C18—C17	178.06 (15)
C14—C19—C10—C11	−0.2 (2)	C19—C18—C17—C16	0.1 (3)
C18—C19—C10—N2	5.3 (2)	C6—C1—C2—C3	0.8 (3)
C14—C19—C10—N2	−176.33 (14)	C13—C14—C15—C16	−178.85 (17)
C5—C6—C1—C2	−1.2 (2)	C19—C14—C15—C16	0.6 (2)
C7—C6—C1—C2	−179.20 (16)	C14—C15—C16—C17	−0.8 (3)
C1—C6—C7—C8	−36.3 (2)	C18—C17—C16—C15	0.4 (3)
C5—C6—C7—C8	145.94 (17)	C6—C7—C8—C9	177.95 (15)
N2—C10—C11—C12	175.23 (16)	N2—C9—C8—C7	175.93 (17)
C19—C10—C11—C12	−0.6 (2)	C1—C2—C3—C4	0.2 (3)
C18—C19—C14—C13	179.40 (15)	C5—C4—C3—C2	−0.8 (3)
C10—C19—C14—C13	1.0 (2)		

Fig. 1


O2
O1
N1
C5
C6
C4
C7
C8
C9
N2
C10
C11
C12
C13
C14
C19
C15
C1
C3
C2
C18
C16
C17