Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(4-Cyanophenyldiazen-2-ium-1-yl)-2-naphtholate

Yan-Hong Yu[a]* and Kun Qian[b]

[a]Jiangxi Key Laboratory of Organic Chemistry, Jiangxi Science and Technology, Normal University, Nanchang 330013, People's Republic of China, and [b]Academic Administration of Jiangxi University of Traditional Chinese, Medicine, NanChang 330047, People's Republic of China
Correspondence e-mail: yuyanhong001@yahoo.com.cn

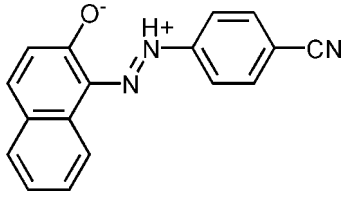
Received 17 July 2009; accepted 18 July 2009

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.054; wR factor = 0.148; data-to-parameter ratio = 15.8.

In the molecule of the zwitterionic title compound, $C_{17}H_{11}N_3O$, the naphthalene ring system is planar [maximum deviation = 0.029 (3) Å] and is oriented at a dihedral angle of 3.55 (3)° with respect to the benzene ring. An intramolecular N—H···O hydrogen bond results in the formation of a planar six-membered ring. In the crystal structure, intermolecular C—H···O interactions link the molecules into centrosymmetric dimers.

Related literature

For general background to azo compounds and their use in dyes, pigments and advanced materials, see: Lee *et al.* (2004); Oueslati *et al.* (2004). For a related structure, see: Rădulescu *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{17}H_{11}N_3O$
M_r = 273.29
Monoclinic, $P2_1/c$
a = 5.2673 (11) Å
b = 9.910 (2) Å
c = 25.239 (6) Å
β = 96.13 (3)°
V = 1309.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 K
0.35 × 0.10 × 0.10 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.973, T_{max} = 0.979
13086 measured reflections
2998 independent reflections
1941 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.148
S = 1.02
2998 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	1.91	2.580 (2)	133
C12—H12A···O1^{i}	0.93	2.45	3.362 (2)	166

Symmetry code: (i) $-x+1, -y, -z+1$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2742).

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.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Lee, S. H., Kim, J. Y., Ko, J., Lee, J. Y. & Kim, J. S. (2004). *J. Org. Chem.* **69**, 2902–2905.
Oueslati, F., Dumazet-Bonnamour, I. & Lamartine, R. (2004). *New J. Chem.* **28**, 1575–1578.
Rădulescu, C., Hossu, A. M. & Ioniţă, I. (2006). *Dyes Pigments*, **71**, 123–129.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2009). E**65**, o2033 [**doi:10.1107/S1600536809028438**]

1-(4-Cyanophenyldiazen-2-ium-1-yl)-2-naphtholate

Y.-H. Yu and K. Qian

Comment

Azo compounds are characterized by the azo linkage (–N=N–) and are very important in the fields of dyes, pigments and advanced materials (Lee *et al.*, 2004; Oueslati *et al.*, 2004). We report herein the crystal structure of the title compound, obtained through the diazotization of 4-aminobenzonitrile followed by a coupling reaction with 2-naphthol.

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (C1-C5/C10), B (C5-C10) and C (C11-C16) are, of course, planar, and they are oriented at dihedral angles of A/B = 2.32 (3), A/C = 2.58 (3) and B/C = 4.59 (3) °. The naphthalene ring system is planar with a maximum deviation of 0.029 (3) Å for atom C5. Intramolecular N-H···O hydrogen bond (Table 1) results in the formation of planar six-membered ring D (O1/N1/N2/C1/C2/H2A), which is oriented with respect to rings A, B and C at dihedral angles of A/D = 1.12 (3), B/D = 3.29 (3) and C/D = 1.47 (3) °. So, rings A, B, C and D are almost coplanar.

In the crystal structure, intermolecular C-H···O interactions link the molecules into centrosymmetric dimers (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

The title compound was prepared according to a literature method (Rădulescu *et al.*, 2006). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Refinement

H atoms were positioned geometrically with N-H = 0.86 Å (for NH) and C-H = 0.93 Å for aromatic H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Figures

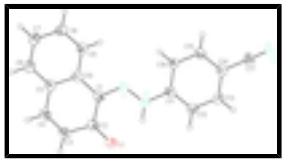


Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Hydrogen bond is shown as dashed line.

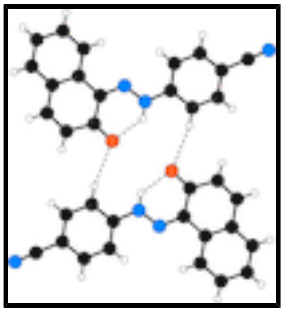


Fig. 2. A partial packing diagram. Hydrogen bonds are shown as dashed lines.

1-(4-Cyanophenyldiazen-2-ium-1-yl)-2-naphtholate

Crystal data

$C_{17}H_{11}N_3O$	$F_{000} = 568$
$M_r = 273.29$	$D_x = 1.386$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1658 reflections
$a = 5.2673$ (11) Å	$\theta = 3.2$–28.9°
$b = 9.910$ (2) Å	$\mu = 0.09$ mm^{-1}
$c = 25.239$ (6) Å	$T = 294$ K
$\beta = 96.13$ (3)°	Block, red
$V = 1309.9$ (5) Å^3	0.35 × 0.10 × 0.10 mm
$Z = 4$	

Data collection

Rigaku SCXmini diffractometer	2998 independent reflections
Radiation source: fine-focus sealed tube	1941 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.059$
Detector resolution: 13.6612 pixels mm^{-1}	$\theta_{max} = 27.5^\circ$
$T = 294$ K	$\theta_{min} = 3.2^\circ$
ω scans	$h = -6 \rightarrow 6$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	$k = -12 \rightarrow 12$
$T_{min} = 0.973$, $T_{max} = 0.979$	$l = -32 \rightarrow 32$
13086 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
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.0861P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
2998 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
190 parameters	$\Delta\rho_{min}$ = −0.25 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	0.2630 (3)	−0.03169 (14)	0.45197 (5)	0.0627 (4)
N1	0.3499 (3)	0.15188 (14)	0.36889 (6)	0.0424 (4)
N2	0.5123 (3)	0.16008 (14)	0.41170 (5)	0.0444 (4)
H2A	0.4994	0.1072	0.4383	0.053*
N3	1.4464 (4)	0.62761 (18)	0.42541 (8)	0.0731 (5)
C1	0.1628 (3)	0.06230 (17)	0.36607 (7)	0.0427 (4)
C2	0.1200 (4)	−0.03101 (18)	0.40895 (7)	0.0503 (5)
C3	−0.0963 (4)	−0.12070 (19)	0.39970 (8)	0.0576 (5)
H3A	−0.1284	−0.1821	0.4261	0.069*
C4	−0.2519 (4)	−0.11777 (18)	0.35418 (8)	0.0542 (5)
H4A	−0.3884	−0.1777	0.3501	0.065*
C5	−0.2179 (3)	−0.02633 (17)	0.31131 (7)	0.0456 (4)
C6	−0.3895 (3)	−0.02176 (19)	0.26515 (7)	0.0534 (5)
H6A	−0.5266	−0.0814	0.2614	0.064*
C7	−0.3597 (4)	0.0688 (2)	0.22535 (7)	0.0554 (5)
H7A	−0.4760	0.0711	0.1949	0.066*
C8	−0.1543 (4)	0.15722 (19)	0.23078 (7)	0.0514 (5)
H8A	−0.1329	0.2185	0.2037	0.062*
C9	0.0175 (3)	0.15515 (18)	0.27562 (7)	0.0474 (4)
H9A	0.1544	0.2149	0.2786	0.057*
C10	−0.0106 (3)	0.06409 (16)	0.31707 (6)	0.0410 (4)
C11	0.7076 (3)	0.25635 (16)	0.41359 (6)	0.0398 (4)
C12	0.8755 (3)	0.26618 (19)	0.45927 (7)	0.0505 (5)
H12A	0.8579	0.2089	0.4878	0.061*
C13	1.0691 (4)	0.36029 (19)	0.46282 (7)	0.0514 (5)
H13A	1.1819	0.3666	0.4937	0.062*
C14	1.0948 (3)	0.44545 (17)	0.42018 (7)	0.0446 (4)

C15	0.9273 (3)	0.43388 (19)	0.37409 (7)	0.0509 (5)
H15A	0.9456	0.4904	0.3453	0.061*
C16	0.7350 (3)	0.33980 (18)	0.37050 (7)	0.0477 (4)
H16A	0.6240	0.3321	0.3394	0.057*
C17	1.2921 (4)	0.5465 (2)	0.42332 (7)	0.0533 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0707 (9)	0.0608 (8)	0.0547 (8)	−0.0102 (7)	−0.0025 (7)	0.0170 (6)
N1	0.0445 (8)	0.0398 (8)	0.0427 (8)	0.0009 (6)	0.0035 (6)	−0.0017 (6)
N2	0.0509 (9)	0.0406 (8)	0.0417 (8)	−0.0023 (6)	0.0044 (7)	0.0056 (6)
N3	0.0691 (11)	0.0661 (12)	0.0849 (14)	−0.0198 (10)	0.0124 (10)	−0.0066 (10)
C1	0.0452 (10)	0.0373 (9)	0.0464 (9)	0.0016 (7)	0.0087 (8)	−0.0003 (7)
C2	0.0557 (11)	0.0443 (10)	0.0515 (11)	0.0010 (8)	0.0091 (9)	0.0054 (8)
C3	0.0612 (12)	0.0487 (11)	0.0638 (12)	−0.0088 (9)	0.0104 (10)	0.0127 (9)
C4	0.0503 (11)	0.0446 (10)	0.0680 (13)	−0.0085 (8)	0.0084 (10)	0.0016 (9)
C5	0.0459 (10)	0.0413 (10)	0.0505 (10)	−0.0009 (8)	0.0100 (8)	−0.0057 (8)
C6	0.0474 (10)	0.0532 (11)	0.0591 (12)	−0.0049 (9)	0.0031 (9)	−0.0092 (9)
C7	0.0531 (11)	0.0616 (12)	0.0501 (11)	0.0027 (10)	−0.0005 (9)	−0.0086 (9)
C8	0.0563 (11)	0.0534 (11)	0.0448 (10)	0.0023 (9)	0.0064 (9)	−0.0002 (8)
C9	0.0486 (10)	0.0461 (10)	0.0481 (10)	−0.0027 (8)	0.0084 (8)	−0.0017 (8)
C10	0.0426 (9)	0.0376 (9)	0.0436 (9)	0.0025 (7)	0.0087 (7)	−0.0034 (7)
C11	0.0425 (9)	0.0354 (9)	0.0421 (9)	0.0019 (7)	0.0080 (7)	−0.0002 (7)
C12	0.0621 (12)	0.0494 (11)	0.0392 (9)	−0.0036 (9)	0.0021 (9)	0.0042 (8)
C13	0.0551 (11)	0.0540 (11)	0.0436 (10)	−0.0057 (9)	−0.0016 (8)	−0.0025 (8)
C14	0.0435 (9)	0.0422 (9)	0.0488 (10)	0.0004 (8)	0.0090 (8)	−0.0023 (8)
C15	0.0520 (11)	0.0498 (10)	0.0517 (10)	−0.0005 (9)	0.0088 (9)	0.0122 (8)
C16	0.0483 (10)	0.0505 (10)	0.0429 (9)	−0.0007 (8)	−0.0007 (8)	0.0074 (8)
C17	0.0523 (11)	0.0541 (11)	0.0543 (11)	−0.0045 (9)	0.0098 (9)	−0.0034 (9)

Geometric parameters (Å, °)

O1—C2	1.254 (2)	C7—C8	1.387 (3)
N1—N2	1.3072 (19)	C7—H7A	0.9300
N1—C1	1.323 (2)	C8—C9	1.372 (2)
N2—C11	1.400 (2)	C8—H8A	0.9300
N2—H2A	0.8600	C9—C10	1.401 (2)
N3—C17	1.141 (2)	C9—H9A	0.9300
C1—C10	1.457 (2)	C11—C12	1.380 (2)
C1—C2	1.459 (2)	C11—C16	1.386 (2)
C2—C3	1.444 (3)	C12—C13	1.378 (2)
C3—C4	1.338 (3)	C12—H12A	0.9300
C3—H3A	0.9300	C13—C14	1.386 (2)
C4—C5	1.437 (3)	C13—H13A	0.9300
C4—H4A	0.9300	C14—C15	1.387 (2)
C5—C6	1.397 (2)	C14—C17	1.439 (3)
C5—C10	1.408 (2)	C15—C16	1.373 (2)
C6—C7	1.369 (3)	C15—H15A	0.9300

C6—H6A	0.9300	C16—H16A	0.9300
N2—N1—C1	120.28 (14)	C7—C8—H8A	119.6
N1—N2—C11	118.95 (14)	C8—C9—C10	120.83 (17)
N1—N2—H2A	120.5	C8—C9—H9A	119.6
C11—N2—H2A	120.5	C10—C9—H9A	119.6
N1—C1—C10	115.69 (15)	C9—C10—C5	118.39 (16)
N1—C1—C2	123.97 (16)	C9—C10—C1	122.33 (15)
C10—C1—C2	120.31 (15)	C5—C10—C1	119.27 (15)
O1—C2—C3	121.83 (17)	C12—C11—C16	120.16 (16)
O1—C2—C1	121.30 (16)	C12—C11—N2	118.66 (15)
C3—C2—C1	116.86 (17)	C16—C11—N2	121.18 (16)
C4—C3—C2	121.70 (18)	C13—C12—C11	120.41 (16)
C4—C3—H3A	119.1	C13—C12—H12A	119.8
C2—C3—H3A	119.1	C11—C12—H12A	119.8
C3—C4—C5	123.09 (17)	C12—C13—C14	119.67 (17)
C3—C4—H4A	118.5	C12—C13—H13A	120.2
C5—C4—H4A	118.5	C14—C13—H13A	120.2
C6—C5—C10	119.42 (16)	C13—C14—C15	119.65 (16)
C6—C5—C4	121.78 (16)	C13—C14—C17	120.72 (17)
C10—C5—C4	118.76 (16)	C15—C14—C17	119.63 (16)
C7—C6—C5	121.22 (17)	C16—C15—C14	120.67 (16)
C7—C6—H6A	119.4	C16—C15—H15A	119.7
C5—C6—H6A	119.4	C14—C15—H15A	119.7
C6—C7—C8	119.42 (18)	C15—C16—C11	119.44 (16)
C6—C7—H7A	120.3	C15—C16—H16A	120.3
C8—C7—H7A	120.3	C11—C16—H16A	120.3
C9—C8—C7	120.72 (18)	N3—C17—C14	179.1 (2)
C9—C8—H8A	119.6		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1	0.86	1.91	2.580 (2)	133
C12—H12A···O1^{i}	0.93	2.45	3.362 (2)	166

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1.

Fig. 1

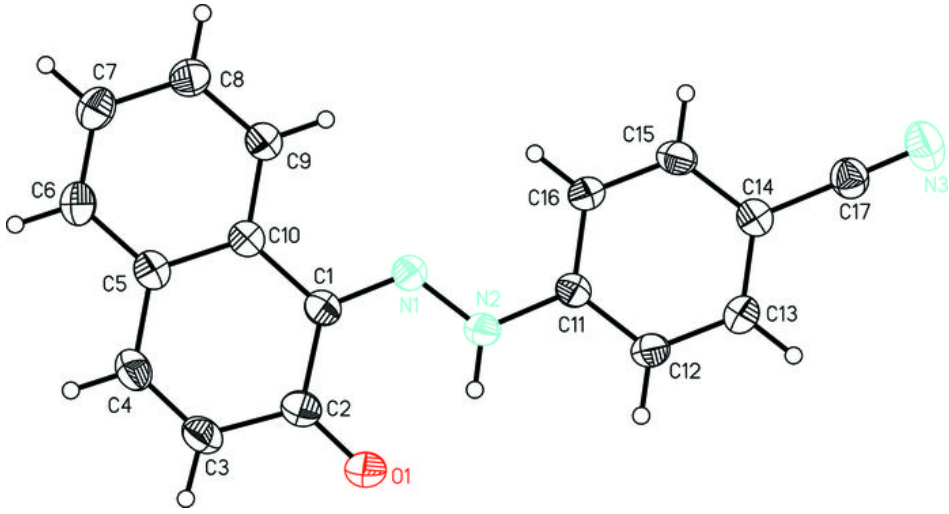

C7
C8
C9
C6
C10
C5
C1
N1
N2
C11
C15
C16
C14
C17
N3
C13
C12
C4
C2
C3
O1

Fig. 2