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(*E*)-1-(2-Phenyldiazen-2-ium-1-yl)naphthalen-2-olate

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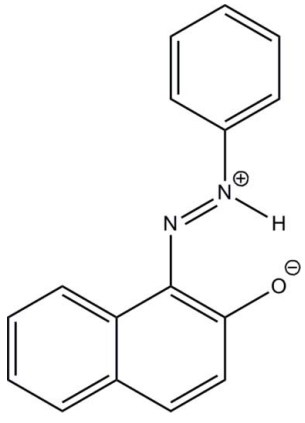
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.054; wR factor = 0.144; data-to-parameter ratio = 12.4.

In the title zwitterionic compound, $C_{16}H_{12}N_2O$, the dihedral angle between the phenyl ring and the naphthalene ring system is 17.85 (8)°; an intramolecular N—H···O hydrogen bond occurs. In the crystal, π–π stacking is observed between naphthalene ring systems of adjacent molecules, the centroid–centroid distance being 3.6486 (11) Å.

Related literature

For general background to azo compounds and their applications in the fields of dyes, pigments and advanced materials, see: Biswas & Umapathy (2000); Willner & Rubin (1996); Hunger (2003); Catino & Farris (1985); Zollinger (2003); Bahatti & Seshadri (2004); Taniike *et al.* (1996); Fadda *et al.* (1994); Bach *et al.* (1996); Clark & Hester (1993). For the synthesis, see: Wang *et al.* (2003).



Experimental

Crystal data

$C_{16}H_{12}N_2O$
M_r = 248.28
Monoclinic, $P2_1/c$
a = 13.0800 (12) Å
b = 13.5170 (13) Å
c = 7.0080 (4) Å
β = 94.140 (6)°
V = 1235.80 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 150 K
0.26 × 0.22 × 0.17 mm

Data collection

Nonius KappaCCD diffractometer
4092 measured reflections
2139 independent reflections
1546 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.144
S = 1.06
2139 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.94	1.73	2.5346 (19)	141

Data collection: *KappaCCD Server Software* (Nonius, 1999); cell refinement: *KappaCCD Server Software*; data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS86* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

The authors would like to thank Professor L. Ouahab, University of Rennes (France), for his valuable collaboration in the recording and interpretation of the XRD data and Professor S. E. Bouaoud, University of Constantine (Algeria) for providing laboratory facilities and encouragement.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5718).

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supporting information

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(*E*)-1-(2-Phenyldiazen-2-ium-1-yl)naphthalen-2-olate

Hassiba Bougueria, Souheyla Chetioui, Issam Boudraa, Abd el kader Bouchoul and Salah Eddine Bouaoud

S1. Comment

Azo compounds are very important in the field of dyes, pigments and advanced materials (Hunger, 2003). It has been known for many years that the azo compounds are the most widely used class of dyes, due to their versatile applications in various fields such as the dyeing of textile fibers, the coloring of different materials, colored plastics and polymers, biological-medical studies and advanced applications in organic syntheses (Catino & Farris, 1985; Zollinger, 2003; Bahatti & Seshadri, 2004; Taniike *et al.*, 1996; Fadda *et al.*, 1994). They are also used in the fields of nonlinear optics and optical data storage (Taniike *et al.*, 1996; Bach *et al.*, 1996; Clark & Hester, 1993). Their optical properties depend on not only the spectroscopic properties of the molecules but also their crystallographic arrangements (Biswas & Umapathy, 2000; Willner & Rubin, 1996).

We report here in the crystal structure of the title compound, obtained through the diazotization of aniline followed by a coupling reaction with 2-naphthol.

The molecule of the title compound, with the atom numbering scheme, is shown in Fig. 1, crystallizes in the monoclinic space group *P*21/*c*.

The molecular structure of C_{16} H_{12} N_2 O is illustrated in Fig. 1. The molecule adopts an anti–configuration with the two aryl groups reside on the opposite side of azo–group. The dihedral angle between the benzene ring and naphthalene ring is 17.85 (8)°. An intramolecular N—H···O hydrogen bond is found (Table 1). It is more interesting, that hydrogen atom in the OH-group has transfer to N atom in the azo-group to form the structure of dipolar ion. Moreover, different Fourier map indicate hydrogen site location is closer to nitrogen atom of azo-group. In the crystal molecules are packed by the weak π–π interactions with the closest approach between centroids of aromatic rings is 3.6486 (11) Å.

S2. Experimental

The compound was synthesized according to the literature procedure of other aromatic azo-compounds (Wang *et al.*, 2003). Red prism of the compound were obtained by slow evaporation at room temperature from an aqueous solution containing water/THF (1/1, v/v).

S3. Refinement

N-bound H atom was located in a differece Fourier map and refined with N—H distance constraint of 0.94 Å, other H atoms were placed in calculated positions and refined in riding mode. U_{iso}(H) = 1.2U_{eq}(N,C).

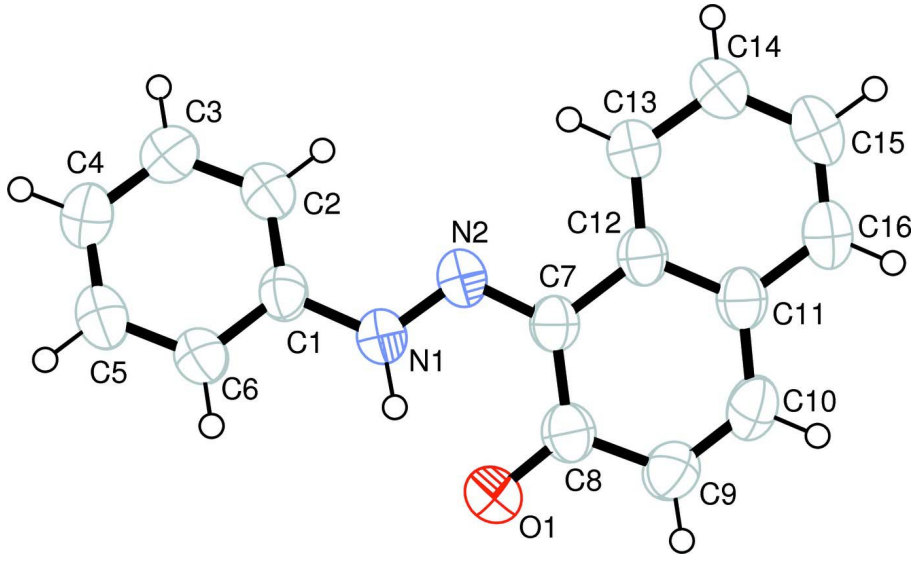

Figure 1

View of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

(*E*)-1-(2-Phenyldiazen-2-ium-1-yl)naphthalen-2-olate

Crystal data

$C_{16}H_{12}N_2O$
$M_r = 248.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.0800\ (12)$ Å
$b = 13.5170\ (13)$ Å
$c = 7.0080\ (4)$ Å
$\beta = 94.140\ (6)°$
$V = 1235.80\ (18)$ Å^3
$Z = 4$
$F(000) = 520$
$D_x = 1.334$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2200 reflections
$\theta = 1.0–25.4°$
$\mu = 0.09$ mm^{-1}
$T = 150$ K
Prism, red
0.26 × 0.22 × 0.17 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
CCD scans
4092 measured reflections
2139 independent reflections
1546 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.4°$, $\theta_{min} = 2.2°$
$h = -15\rightarrow15$
$k = -16\rightarrow16$
$l = -7\rightarrow7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.144$
$S = 1.06$
2139 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0756P)^2 + 0.113P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

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

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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}
N1	0.20061 (11)	0.46423 (10)	0.4042 (2)	0.0542 (4)
H1	0.1287	0.4666	0.4047	0.065*
N2	0.23990 (12)	0.37596 (10)	0.4036 (2)	0.0524 (4)
O1	0.02112 (10)	0.39323 (10)	0.3599 (2)	0.0688 (4)
C1	0.26520 (14)	0.54729 (12)	0.4226 (2)	0.0510 (4)
C2	0.36888 (15)	0.54252 (15)	0.3965 (3)	0.0630 (5)
H2	0.3987	0.4832	0.3627	0.076*
C3	0.42736 (16)	0.62723 (15)	0.4215 (3)	0.0700 (6)
H3	0.4972	0.6246	0.4052	0.084*
C4	0.38374 (17)	0.71530 (16)	0.4701 (3)	0.0727 (6)
H4	0.4240	0.7718	0.4868	0.087*
C5	0.28076 (17)	0.71967 (15)	0.4938 (3)	0.0718 (6)
H5	0.2511	0.7792	0.5267	0.086*
C6	0.22090 (15)	0.63589 (13)	0.4690 (3)	0.0603 (5)
H6	0.1509	0.6392	0.4836	0.072*
C7	0.17482 (13)	0.29843 (12)	0.3881 (2)	0.0490 (4)
C8	0.06510 (15)	0.30859 (14)	0.3645 (3)	0.0563 (5)
C9	0.00491 (15)	0.22000 (16)	0.3455 (3)	0.0651 (5)
H9	−0.0660	0.2249	0.3272	0.078*
C10	0.04871 (16)	0.12996 (15)	0.3537 (3)	0.0634 (5)
H10	0.0069	0.0744	0.3419	0.076*
C11	0.15749 (15)	0.11656 (13)	0.3798 (2)	0.0543 (5)
C12	0.22131 (14)	0.20077 (12)	0.3962 (2)	0.0509 (4)
C13	0.32739 (15)	0.18637 (15)	0.4207 (3)	0.0635 (5)
H13	0.3709	0.2408	0.4328	0.076*
C14	0.36788 (17)	0.09244 (15)	0.4270 (3)	0.0728 (6)
H14	0.4385	0.0840	0.4437	0.087*
C15	0.30467 (18)	0.01006 (16)	0.4088 (3)	0.0723 (6)
H15	0.3329	−0.0531	0.4119	0.087*
C16	0.20132 (17)	0.02215 (14)	0.3865 (3)	0.0647 (5)
H16	0.1591	−0.0332	0.3755	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0545 (9)	0.0442 (9)	0.0639 (10)	0.0000 (7)	0.0040 (7)	0.0008 (6)
N2	0.0613 (9)	0.0424 (9)	0.0534 (9)	0.0008 (7)	0.0040 (6)	−0.0001 (6)
O1	0.0601 (8)	0.0556 (9)	0.0902 (10)	0.0066 (7)	0.0019 (7)	−0.0011 (7)
C1	0.0580 (10)	0.0412 (10)	0.0534 (10)	−0.0017 (8)	0.0010 (8)	0.0031 (7)
C2	0.0625 (12)	0.0510 (12)	0.0760 (13)	0.0055 (9)	0.0072 (9)	−0.0013 (9)
C3	0.0567 (11)	0.0630 (14)	0.0899 (15)	−0.0042 (10)	0.0027 (10)	0.0022 (10)
C4	0.0723 (14)	0.0514 (12)	0.0939 (16)	−0.0106 (11)	0.0019 (11)	−0.0008 (10)
C5	0.0777 (14)	0.0455 (11)	0.0925 (16)	0.0029 (10)	0.0086 (11)	−0.0029 (10)
C6	0.0580 (11)	0.0488 (11)	0.0743 (13)	0.0035 (9)	0.0071 (9)	0.0036 (9)
C7	0.0558 (10)	0.0446 (10)	0.0466 (10)	−0.0025 (8)	0.0039 (7)	−0.0027 (7)
C8	0.0641 (12)	0.0525 (11)	0.0523 (11)	−0.0002 (9)	0.0044 (8)	−0.0025 (8)
C9	0.0586 (11)	0.0626 (13)	0.0739 (13)	−0.0071 (10)	0.0031 (9)	−0.0106 (9)
C10	0.0699 (13)	0.0528 (12)	0.0679 (12)	−0.0153 (10)	0.0065 (9)	−0.0085 (9)
C11	0.0702 (12)	0.0464 (11)	0.0467 (10)	−0.0040 (9)	0.0061 (8)	−0.0048 (7)
C12	0.0628 (11)	0.0451 (10)	0.0450 (10)	−0.0017 (8)	0.0059 (7)	−0.0012 (7)
C13	0.0623 (12)	0.0501 (12)	0.0780 (13)	−0.0001 (9)	0.0039 (10)	0.0015 (9)
C14	0.0701 (13)	0.0554 (13)	0.0928 (16)	0.0097 (11)	0.0050 (11)	0.0043 (11)
C15	0.0933 (16)	0.0450 (12)	0.0788 (14)	0.0100 (11)	0.0081 (11)	0.0016 (9)
C16	0.0843 (14)	0.0447 (11)	0.0654 (12)	−0.0052 (10)	0.0079 (10)	−0.0032 (8)

Geometric parameters (Å, º)

N1—N2	1.2993 (19)	C7—C12	1.453 (2)
N1—C1	1.405 (2)	C8—C9	1.434 (3)
N1—H1	0.9418	C9—C10	1.345 (3)
N2—C7	1.350 (2)	C9—H9	0.9300
O1—C8	1.280 (2)	C10—C11	1.433 (3)
C1—C6	1.380 (2)	C10—H10	0.9300
C1—C2	1.383 (3)	C11—C16	1.398 (3)
C2—C3	1.381 (3)	C11—C12	1.411 (2)
C2—H2	0.9300	C12—C13	1.399 (3)
C3—C4	1.374 (3)	C13—C14	1.375 (3)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.370 (3)	C14—C15	1.387 (3)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.381 (3)	C15—C16	1.359 (3)
C5—H5	0.9300	C15—H15	0.9300
C6—H6	0.9300	C16—H16	0.9300
C7—C8	1.439 (3)		
N2—N1—C1	119.91 (15)	O1—C8—C7	122.06 (16)
N2—N1—H1	115.2	C9—C8—C7	117.85 (17)
C1—N1—H1	124.6	C10—C9—C8	121.51 (18)
N1—N2—C7	117.78 (15)	C10—C9—H9	119.2
C6—C1—C2	120.28 (17)	C8—C9—H9	119.2

C6—C1—N1	117.08 (16)	C9—C10—C11	122.41 (18)
C2—C1—N1	122.64 (16)	C9—C10—H10	118.8
C3—C2—C1	118.96 (18)	C11—C10—H10	118.8
C3—C2—H2	120.5	C16—C11—C12	119.65 (18)
C1—C2—H2	120.5	C16—C11—C10	121.37 (17)
C4—C3—C2	120.9 (2)	C12—C11—C10	118.98 (16)
C4—C3—H3	119.5	C13—C12—C11	118.24 (16)
C2—C3—H3	119.5	C13—C12—C7	122.67 (16)
C5—C4—C3	119.80 (19)	C11—C12—C7	119.09 (17)
C5—C4—H4	120.1	C14—C13—C12	120.57 (18)
C3—C4—H4	120.1	C14—C13—H13	119.7
C4—C5—C6	120.19 (19)	C12—C13—H13	119.7
C4—C5—H5	119.9	C13—C14—C15	120.8 (2)
C6—C5—H5	119.9	C13—C14—H14	119.6
C1—C6—C5	119.85 (18)	C15—C14—H14	119.6
C1—C6—H6	120.1	C16—C15—C14	119.7 (2)
C5—C6—H6	120.1	C16—C15—H15	120.2
N2—C7—C8	123.58 (16)	C14—C15—H15	120.2
N2—C7—C12	116.27 (16)	C15—C16—C11	121.02 (19)
C8—C7—C12	120.16 (16)	C15—C16—H16	119.5
O1—C8—C9	120.09 (18)	C11—C16—H16	119.5

C1—N1—N2—C7	179.15 (14)	C8—C9—C10—C11	−0.6 (3)
N2—N1—C1—C6	−164.58 (16)	C9—C10—C11—C16	−179.56 (17)
N2—N1—C1—C2	15.3 (2)	C9—C10—C11—C12	−0.5 (3)
C6—C1—C2—C3	1.3 (3)	C16—C11—C12—C13	−0.6 (2)
N1—C1—C2—C3	−178.58 (17)	C10—C11—C12—C13	−179.67 (16)
C1—C2—C3—C4	−0.5 (3)	C16—C11—C12—C7	179.69 (14)
C2—C3—C4—C5	−0.2 (3)	C10—C11—C12—C7	0.6 (2)
C3—C4—C5—C6	0.0 (3)	N2—C7—C12—C13	0.7 (2)
C2—C1—C6—C5	−1.5 (3)	C8—C7—C12—C13	−179.37 (16)
N1—C1—C6—C5	178.41 (17)	N2—C7—C12—C11	−179.68 (14)
C4—C5—C6—C1	0.8 (3)	C8—C7—C12—C11	0.3 (2)
N1—N2—C7—C8	2.6 (2)	C11—C12—C13—C14	0.5 (3)
N1—N2—C7—C12	−177.42 (13)	C7—C12—C13—C14	−179.82 (17)
N2—C7—C8—O1	−1.2 (3)	C12—C13—C14—C15	0.1 (3)
C12—C7—C8—O1	178.80 (15)	C13—C14—C15—C16	−0.7 (3)
N2—C7—C8—C9	178.63 (15)	C14—C15—C16—C11	0.6 (3)
C12—C7—C8—C9	−1.3 (2)	C12—C11—C16—C15	0.1 (3)
O1—C8—C9—C10	−178.64 (17)	C10—C11—C16—C15	179.11 (18)
C7—C8—C9—C10	1.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.94	1.73	2.5346 (19)	141