Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(4-Methylphenyldiazoniumyl)-2-naphtholate

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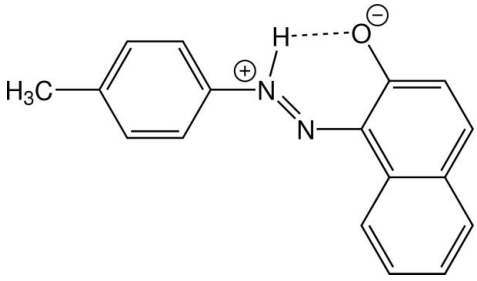
Received 23 November 2007; accepted 29 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.053; wR factor = 0.149; data-to-parameter ratio = 15.7.

In the title compound, $C_{17}H_{14}N_2O$, the dihedral angle between the benzene ring and naphthalene ring system is 11.0 (3)°. The azo group adopts an *anti* configuration and an intramolecular N—H···O hydrogen bond exists. Molecules are packed by π–π interactions between adjacent molecule (closest approach between centroids of benzene and naphthalene rings of 3.501 Å).

Related literature

For related literature, see: Lee *et al.* (2004); Oueslati *et al.* (2004); Wang *et al.* (2003).



Experimental

Crystal data

$C_{17}H_{14}N_2O$
M_r = 262.30
Monoclinic, $P2_1/c$
a = 13.6740 (4) Å
b = 13.8000 (4) Å
c = 7.1430 (2) Å
β = 95.752 (2)°
V = 1341.11 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.984, T_{max} = 0.992
14681 measured reflections
2913 independent reflections
1802 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.149
S = 1.04
2913 reflections
185 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 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
N1—H1A···O1	1.078 (16)	1.578 (16)	2.5414 (16)	145.5 (12)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

We gratefully acknowledge the financial support of the National Science Funds for Distinguished Young Scholars of Hubei Province, People's Republic of China (Grant No. 2006ABB038), the Outstanding Mid-Young Scholars' Programs, Hubei Provincial Department of Education (Q20072203) and the Project sponsored by SRF for ROCS, SEM (200724).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HJ2006).

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supplementary materials

Acta Cryst. (2008). E**64**, o218 [**doi:10.1107/S1600536807064549**]

1-(4-Methylphenyldiazoniumyl)-2-naphtholate

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Comment

Azo compounds are very important in the fields of dyes, pigments and advanced materials (Lee *et al.*, 2004; Oueslati *et al.*, 2004). Azo dyes are synthetic colours that contain an azo group, as part of the structure. Azo groups do not occur naturally. Many azo compounds have been synthesized by the diazotization and diazo coupling reaction (Wang *et al.*, 2003). The title compound (I) was obtained through the diazotization of 4-methylaniline followed by a coupling reaction with 2-naphthol.

The molecular structure of the title compound is illustrated in figure 1, where the molecule adopts an anti configuration with the two aryl groups residing on the opposite sides of azo group. The dihedral angle between the benzene ring and naphthalene ring is 11.0 (3)°. An intramolecular N—H···O hydrogen bond exists in each molecule (Table 1). Interestingly, the hydrogen atom in the OH group has transfer to the N atom in the azo group to form a dipolar ion; the difference Fourier map indicated that the hydrogen site location is closer to nitrogen atom of the azo group. The molecules are packed by the π···π interactions with the closest approach between centroids of aromatic rings of 3.501Å (symmetry equivalent x, $-y+1$, $z-1/2$).

Experimental

The title compound was prepared by a similar method of other aromatic azo compounds(Wang *et al.*, 2003). Single crystals of (I) were obtained by slow evaporation from a petroleum ether-ethyl acetate (2:1 *v*/*v*) solution system.

Refinement

H atoms were positioned geometrically at distances of 0.93 (CH), and 0.96Å (CH_3) from the parent C atoms, a riding model was used during the refinement process. The U_{iso} values were constrained to be $1.2U_{eq}$ of the carrier atom, except for methyl H atoms that were constrained to 1.5Ueq of the C atom.

Figures

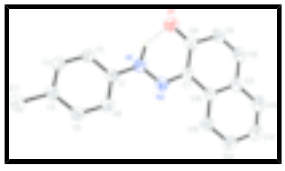

Fig. 1. The structure of (I) showing the atom-numbering with Displacement ellipsoids are drawn at the 30% probability level. The intramolecular H bonded is shown with a dashed line.

-(4-Methylphenyldiazoniumyl)-2-naphtholate

Crystal data

$C_{17}H_{14}N_2O$ $F_{000} = 552$

M_r = 262.30	D_x = 1.299 Mg m^{-3}
Monoclinic, $P2(1)/c$	Melting point: 407 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 13.6740 (4) Å	Cell parameters from 2246 reflections
b = 13.8000 (4) Å	θ = 3.0–23.4º
c = 7.1430 (2) Å	μ = 0.08 mm^{-1}
β = 95.752 (2)º	T = 293 (2) K
V = 1341.11 (7) Å^3	Needle, red
Z = 4	0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART Apex CCD area detector diffractometer	2913 independent reflections
Radiation source: fine-focus sealed tube	1802 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 293(2) K	θ_{max} = 27.0º
phi and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −17→17
T_{min} = 0.984, T_{max} = 0.992	k = −17→16
14681 measured reflections	l = −9→9

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0816P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.053	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.149	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
2913 reflections	Extinction correction: none
185 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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}
C1	0.75809 (11)	−0.03170 (11)	0.1047 (2)	0.0516 (4)
C2	0.72115 (12)	−0.12434 (12)	0.0942 (3)	0.0649 (5)
H2	0.6535	−0.1342	0.0835	0.078*
C3	0.78410 (13)	−0.20284 (12)	0.0996 (3)	0.0687 (5)
H3	0.7580	−0.2651	0.0942	0.082*
C4	0.88439 (12)	−0.19111 (12)	0.1126 (2)	0.0574 (4)
C5	0.91975 (12)	−0.09723 (12)	0.1207 (2)	0.0641 (5)
H5	0.9873	−0.0872	0.1286	0.077*
C6	0.85837 (11)	−0.01801 (12)	0.1176 (2)	0.0611 (5)
H6	0.8844	0.0443	0.1241	0.073*
C7	0.65467 (11)	0.20510 (11)	0.1130 (2)	0.0508 (4)
C8	0.55267 (12)	0.18838 (12)	0.1327 (2)	0.0581 (4)
C9	0.49147 (13)	0.27144 (14)	0.1539 (2)	0.0689 (5)
H9	0.4253	0.2625	0.1690	0.083*
C10	0.52800 (13)	0.36158 (13)	0.1524 (2)	0.0689 (5)
H10	0.4860	0.4135	0.1667	0.083*
C11	0.62899 (12)	0.38124 (11)	0.1296 (2)	0.0580 (4)
C12	0.66538 (15)	0.47637 (13)	0.1275 (3)	0.0735 (5)
H12	0.6234	0.5282	0.1419	0.088*
C13	0.76133 (15)	0.49346 (13)	0.1045 (3)	0.0803 (6)
H13	0.7848	0.5567	0.1042	0.096*
C14	0.82436 (14)	0.41645 (13)	0.0816 (3)	0.0744 (5)
H14	0.8898	0.4284	0.0642	0.089*
C15	0.79103 (12)	0.32326 (12)	0.0843 (2)	0.0638 (5)
H15	0.8343	0.2725	0.0696	0.077*
C16	0.69297 (11)	0.30295 (11)	0.1089 (2)	0.0522 (4)
C17	0.95297 (13)	−0.27743 (13)	0.1212 (3)	0.0742 (5)
H17A	0.9433	−0.3159	0.2298	0.111*
H17B	1.0198	−0.2552	0.1295	0.111*
H17C	0.9393	−0.3159	0.0097	0.111*
N1	0.69010 (9)	0.04469 (9)	0.10377 (18)	0.0561 (4)
H1A	0.6116 (12)	0.0421 (10)	0.109 (2)	0.067*
N2	0.72155 (9)	0.13342 (9)	0.10388 (17)	0.0531 (4)
O1	0.51595 (8)	0.10306 (8)	0.13228 (18)	0.0726 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0530 (9)	0.0517 (9)	0.0499 (9)	0.0026 (7)	0.0044 (7)	0.0032 (7)

C2	0.0512 (9)	0.0586 (11)	0.0846 (13)	−0.0007 (8)	0.0055 (8)	0.0000 (9)
C3	0.0636 (11)	0.0507 (10)	0.0915 (14)	−0.0012 (8)	0.0071 (9)	−0.0010 (9)
C4	0.0636 (11)	0.0586 (11)	0.0506 (10)	0.0090 (8)	0.0090 (7)	0.0010 (7)
C5	0.0497 (9)	0.0699 (12)	0.0732 (12)	0.0028 (8)	0.0089 (8)	0.0042 (9)
C6	0.0538 (9)	0.0549 (10)	0.0749 (12)	−0.0034 (8)	0.0084 (8)	0.0030 (8)
C7	0.0528 (9)	0.0539 (10)	0.0449 (9)	0.0069 (7)	0.0005 (7)	0.0001 (7)
C8	0.0580 (10)	0.0647 (11)	0.0511 (10)	0.0056 (8)	0.0030 (7)	0.0014 (8)
C9	0.0545 (10)	0.0796 (13)	0.0727 (12)	0.0137 (9)	0.0069 (8)	−0.0056 (9)
C10	0.0704 (12)	0.0710 (12)	0.0646 (12)	0.0213 (9)	0.0029 (9)	−0.0069 (9)
C11	0.0690 (11)	0.0560 (10)	0.0471 (9)	0.0095 (8)	−0.0028 (7)	−0.0016 (7)
C12	0.0913 (14)	0.0554 (11)	0.0708 (12)	0.0138 (10)	−0.0060 (10)	−0.0029 (9)
C13	0.0980 (15)	0.0557 (12)	0.0844 (14)	−0.0077 (10)	−0.0045 (11)	0.0005 (9)
C14	0.0726 (12)	0.0633 (12)	0.0858 (13)	−0.0067 (9)	0.0014 (9)	0.0053 (10)
C15	0.0634 (11)	0.0575 (11)	0.0697 (12)	0.0017 (8)	0.0022 (8)	0.0010 (8)
C16	0.0571 (10)	0.0551 (10)	0.0430 (8)	0.0065 (7)	−0.0020 (7)	0.0000 (7)
C17	0.0766 (12)	0.0733 (12)	0.0735 (12)	0.0201 (9)	0.0111 (9)	−0.0002 (9)
N1	0.0504 (8)	0.0528 (9)	0.0650 (9)	0.0024 (6)	0.0056 (6)	0.0043 (6)
N2	0.0571 (8)	0.0510 (8)	0.0507 (8)	0.0023 (6)	0.0034 (6)	0.0015 (6)
O1	0.0574 (7)	0.0664 (8)	0.0945 (10)	−0.0048 (6)	0.0099 (6)	0.0028 (6)

Geometric parameters (Å, °)

C1—C2	1.374 (2)	C9—H9	0.9300
C1—C6	1.378 (2)	C10—C11	1.432 (2)
C1—N1	1.4051 (19)	C10—H10	0.9300
C2—C3	1.382 (2)	C11—C12	1.405 (2)
C2—H2	0.9300	C11—C16	1.407 (2)
C3—C4	1.375 (2)	C12—C13	1.359 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.382 (2)	C13—C14	1.388 (3)
C4—C17	1.513 (2)	C13—H13	0.9300
C5—C6	1.377 (2)	C14—C15	1.365 (2)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—C16	1.398 (2)
C7—N2	1.3531 (18)	C15—H15	0.9300
C7—C8	1.435 (2)	C17—H17A	0.9600
C7—C16	1.450 (2)	C17—H17B	0.9600
C8—O1	1.2799 (18)	C17—H17C	0.9600
C8—C9	1.436 (2)	N1—N2	1.2978 (16)
C9—C10	1.341 (2)	N1—H1A	1.078 (16)
C2—C1—C6	119.29 (14)	C11—C10—H10	118.6
C2—C1—N1	117.28 (14)	C12—C11—C16	119.45 (16)
C6—C1—N1	123.43 (14)	C12—C11—C10	121.66 (15)
C1—C2—C3	120.22 (15)	C16—C11—C10	118.89 (15)
C1—C2—H2	119.9	C13—C12—C11	120.72 (17)
C3—C2—H2	119.9	C13—C12—H12	119.6
C4—C3—C2	121.60 (15)	C11—C12—H12	119.6
C4—C3—H3	119.2	C12—C13—C14	119.98 (17)
C2—C3—H3	119.2	C12—C13—H13	120.0

C3—C4—C5	117.10 (14)	C14—C13—H13	120.0
C3—C4—C17	121.33 (15)	C15—C14—C13	120.49 (18)
C5—C4—C17	121.56 (15)	C15—C14—H14	119.8
C6—C5—C4	122.24 (15)	C13—C14—H14	119.8
C6—C5—H5	118.9	C14—C15—C16	121.10 (16)
C4—C5—H5	118.9	C14—C15—H15	119.5
C5—C6—C1	119.54 (15)	C16—C15—H15	119.5
C5—C6—H6	120.2	C15—C16—C11	118.26 (15)
C1—C6—H6	120.2	C15—C16—C7	122.84 (14)
N2—C7—C8	123.75 (14)	C11—C16—C7	118.90 (14)
N2—C7—C16	115.64 (13)	C4—C17—H17A	109.5
C8—C7—C16	120.57 (14)	C4—C17—H17B	109.5
O1—C8—C7	122.20 (14)	H17A—C17—H17B	109.5
O1—C8—C9	120.12 (15)	C4—C17—H17C	109.5
C7—C8—C9	117.68 (15)	H17A—C17—H17C	109.5
C10—C9—C8	121.20 (16)	H17B—C17—H17C	109.5
C10—C9—H9	119.4	N2—N1—C1	119.26 (13)
C8—C9—H9	119.4	N2—N1—H1A	111.2 (8)
C9—C10—C11	122.74 (15)	C1—N1—H1A	129.5 (8)
C9—C10—H10	118.6	N1—N2—C7	117.67 (13)
C6—C1—C2—C3	1.0 (3)	C10—C11—C12—C13	−179.58 (17)
N1—C1—C2—C3	−178.25 (14)	C11—C12—C13—C14	0.4 (3)
C1—C2—C3—C4	−1.0 (3)	C12—C13—C14—C15	−0.9 (3)
C2—C3—C4—C5	0.2 (3)	C13—C14—C15—C16	0.4 (3)
C2—C3—C4—C17	179.13 (15)	C14—C15—C16—C11	0.4 (2)
C3—C4—C5—C6	0.5 (3)	C14—C15—C16—C7	−179.87 (15)
C17—C4—C5—C6	−178.43 (15)	C12—C11—C16—C15	−0.8 (2)
C4—C5—C6—C1	−0.4 (3)	C10—C11—C16—C15	179.18 (14)
C2—C1—C6—C5	−0.3 (2)	C12—C11—C16—C7	179.46 (14)
N1—C1—C6—C5	178.88 (14)	C10—C11—C16—C7	−0.6 (2)
N2—C7—C8—O1	−4.1 (2)	N2—C7—C16—C15	4.2 (2)
C16—C7—C8—O1	178.26 (13)	C8—C7—C16—C15	−178.03 (14)
N2—C7—C8—C9	175.69 (14)	N2—C7—C16—C11	−176.08 (12)
C16—C7—C8—C9	−1.9 (2)	C8—C7—C16—C11	1.7 (2)
O1—C8—C9—C10	−179.15 (15)	C2—C1—N1—N2	−176.56 (13)
C7—C8—C9—C10	1.0 (2)	C6—C1—N1—N2	4.2 (2)
C8—C9—C10—C11	0.1 (3)	C1—N1—N2—C7	−176.60 (12)
C9—C10—C11—C12	179.64 (16)	C8—C7—N2—N1	3.5 (2)
C9—C10—C11—C16	−0.3 (2)	C16—C7—N2—N1	−178.79 (12)
C16—C11—C12—C13	0.4 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1	1.078 (16)	1.578 (16)	2.5414 (16)	145.5 (12)

Fig. 1