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(*E*)-1-(4-Fluorophenyl)-2-(2-oxidonaphthalen-1-yl)diazenium

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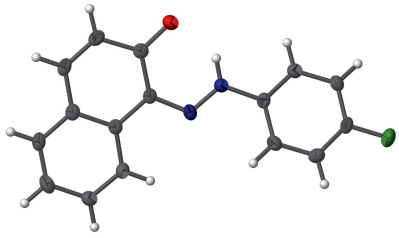
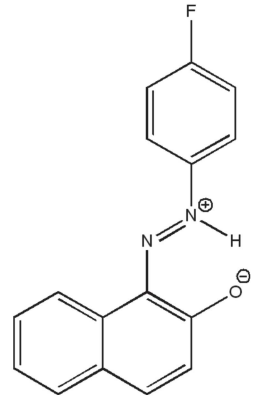
Structural data: full structural data are available from iucrdata.iucr.org

In the title zwitterion, $C_{16}H_{11}FN_2O$, which belongs to the family of azo dyes, the dihedral angle between the benzene ring and the naphthalene ring system is 15.33 (7)° and an intramolecular N—H···O hydrogen bond closes an $S(6)$ ring. In the crystal, inversion dimers linked by weak C—H···O hydrogen bonds generate $R_2^2(16)$ loops. Aromatic π–π stacking [centroid–centroid distance = 3.585 (11) Å] is also observed.

3D view



Chemical scheme



Structure description

The structures and properties of azo dyes (solubility, habit, stability, colour) are dependent on their solid-state structures (Kennedy *et al.*, 2004). As part of our studies in this area, we now describe the structure of the title compound, which shows zwitterionic behaviour (*i.e.* proton transfer from the naphthol group to the azo group) in the solid state.

The dihedral angle between the benzene ring and the naphthalene ring system is 15.33 (7)° and an intramolecular N—H···O hydrogen bond (Fig. 1 and Table 1) closes an $S(6)$ ring. In the crystal, inversion dimers linked by weak C—H···O hydrogen bonds generate $R_2^2(16)$ loops. The dimers are linked through π–π stacking between the benzene ring and naphthalene ring systems of adjacent molecules, the centroid–centroid distance between the C1-ring and C9-ring being 3.585 (11) Å.

Synthesis and crystallization

The title compound was obtained through the diazotization of 4-fluoroaniline followed by a coupling reaction with 2-naphthol according to the established procedure (Wang *et*

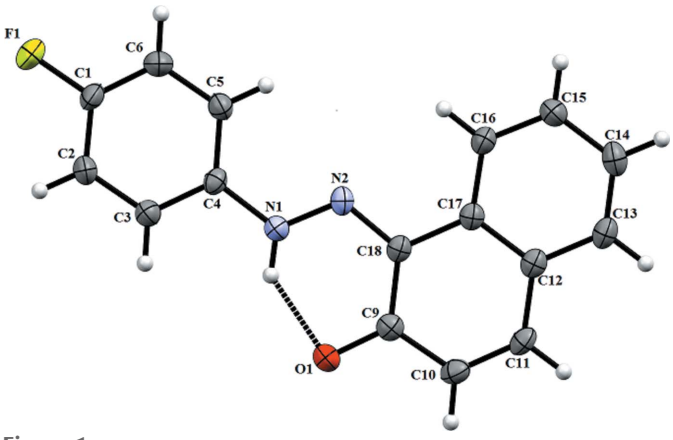


Figure 1
The molecular structure with displacement ellipsoids drawn at the 50% probability level.

al., 2003). Colourless prisms of were obtained by slow evaporation of THF–H_2O (1:1 *v*/*v*) solution at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

We thank all researchers of the CHEMS Research Unit of the University of Constantine Algeria for the valuable assistance they have provided us throughout the realization of this work.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1	0.86	1.83	2.5342 (18)	138
C3—H3···O1^{i}	0.93	2.54	3.417 (2)	157

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{11}FN_2O$
M_r	266.27
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	13.211 (3), 13.685 (2), 6.8580 (14)
β (°)	92.971 (11)
V (Å^3)	1238.2 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.1 × 0.1 × 0.1
Data collection	
Diffractometer	Bruker APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2006)
T_{min}, T_{max}	0.990, 0.990
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10648, 2815, 1886
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.124, 0.97
No. of reflections	2817
No. of parameters	182
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.19

Computer programs: *APEX2* and *SAINT* (Bruker, 2006), *SHELXS86* and *SHELXL97* (Sheldrick, 2008) and *ORTEP-3 for Windows* (Farrugia, 2012).

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full crystallographic data

IUCrData (2017). **2**, x170039 [https://doi.org/10.1107/S2414314617000396]

(*E*)-1-(4-Fluorophenyl)-2-(2-oxidonaphthalen-1-yl)diazen-1-ium

Hassiba Bougueria, Souheyla Chetioui, Assia Mili, Salah eddine Bouaoud and Hocine Merazig

(*E*)-1-(4-Fluorophenyl)-2-(2-oxidonaphthalen-1-yl)diazen-1-ium

Crystal data

$C_{16}H_{11}FN_2O$
M_r = 266.27
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 13.211 (3) Å
b = 13.685 (2) Å
c = 6.8580 (14) Å
β = 92.971 (11)°
V = 1238.2 (4) Å^3
Z = 4
$F(000)$ = 552
D_x = 1.428 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2528 reflections
θ = 3.0–27.1°
μ = 0.10 mm^{-1}
T = 293 K
Prism, colourless
0.1 × 0.1 × 0.1 mm

Data collection

Bruker APEXII diffractometer
Graphite monochromator
CCD rotation images, thin slices scans
Absorption correction: multi-scan (SADABS; Bruker, 2006)
T_{min} = 0.990, T_{max} = 0.990
10648 measured reflections
2815 independent reflections
1886 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −15→17
k = −17→13
l = −8→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.124
S = 0.97
2817 reflections
182 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0721P)^2 + 0.0881P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.06264 (7)	0.21274 (7)	0.05713 (17)	0.0439 (4)
O1	0.48253 (8)	0.60742 (7)	0.13349 (17)	0.0293 (4)
N1	0.30356 (10)	0.54101 (8)	0.09440 (18)	0.0228 (4)
N2	0.26550 (10)	0.62815 (8)	0.09470 (18)	0.0218 (4)
C1	0.12128 (12)	0.29487 (11)	0.0642 (3)	0.0280 (5)
C2	0.22314 (12)	0.28554 (11)	0.0370 (3)	0.0290 (5)
C3	0.28263 (12)	0.36936 (11)	0.0479 (2)	0.0259 (5)
C4	0.23846 (11)	0.45913 (10)	0.0844 (2)	0.0216 (4)
C5	0.13491 (12)	0.46609 (11)	0.1111 (2)	0.0261 (5)
C6	0.07590 (13)	0.38305 (11)	0.1005 (3)	0.0290 (5)
C9	0.44015 (12)	0.69218 (11)	0.1297 (2)	0.0232 (5)
C10	0.50143 (12)	0.77902 (11)	0.1477 (2)	0.0276 (5)
C11	0.45942 (12)	0.86927 (11)	0.1419 (2)	0.0259 (5)
C12	0.35172 (12)	0.88390 (10)	0.1183 (2)	0.0227 (5)
C13	0.30979 (13)	0.97866 (11)	0.1140 (2)	0.0267 (5)
C14	0.20713 (13)	0.99159 (11)	0.0913 (2)	0.0300 (5)
C15	0.14335 (12)	0.91015 (11)	0.0711 (2)	0.0286 (5)
C16	0.18212 (12)	0.81701 (11)	0.0766 (2)	0.0258 (5)
C17	0.28710 (12)	0.80125 (10)	0.1012 (2)	0.0209 (5)
C18	0.33171 (11)	0.70416 (10)	0.1080 (2)	0.0205 (4)
H1N	0.36822	0.53301	0.10028	0.0274*
H2	0.25148	0.22489	0.01198	0.0348*
H3	0.35187	0.36530	0.03071	0.0311*
H5	0.10579	0.52639	0.13602	0.0313*
H6	0.00662	0.38655	0.11756	0.0347*
H10	0.57148	0.77297	0.16368	0.0331*
H11	0.50162	0.92359	0.15343	0.0311*
H13	0.35220	1.03278	0.12652	0.0320*
H14	0.17985	1.05425	0.08938	0.0360*
H15	0.07371	0.91924	0.05368	0.0343*
H16	0.13844	0.76383	0.06400	0.0309*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0319 (6)	0.0280 (5)	0.0717 (8)	−0.0104 (4)	0.0010 (5)	−0.0031 (5)
O1	0.0253 (6)	0.0244 (6)	0.0381 (7)	0.0032 (5)	0.0011 (5)	0.0011 (5)
N1	0.0210 (7)	0.0209 (7)	0.0265 (7)	0.0009 (5)	0.0008 (5)	0.0009 (5)
N2	0.0278 (8)	0.0183 (7)	0.0194 (7)	0.0002 (5)	0.0015 (5)	−0.0003 (5)
C1	0.0265 (9)	0.0210 (8)	0.0360 (9)	−0.0070 (7)	−0.0019 (7)	0.0014 (7)
C2	0.0284 (9)	0.0189 (8)	0.0398 (10)	0.0022 (7)	0.0018 (8)	−0.0008 (7)
C3	0.0237 (9)	0.0239 (8)	0.0301 (9)	0.0009 (6)	0.0021 (7)	0.0020 (6)
C4	0.0245 (8)	0.0206 (7)	0.0194 (8)	−0.0029 (6)	−0.0008 (6)	0.0021 (6)
C5	0.0267 (9)	0.0216 (8)	0.0299 (9)	0.0036 (7)	0.0009 (7)	−0.0009 (6)
C6	0.0214 (8)	0.0295 (9)	0.0360 (10)	0.0000 (7)	0.0012 (7)	−0.0002 (7)

C9	0.0247 (9)	0.0253 (8)	0.0197 (8)	0.0003 (7)	0.0023 (6)	0.0006 (6)
C10	0.0225 (8)	0.0312 (9)	0.0289 (9)	−0.0045 (7)	0.0005 (7)	−0.0041 (7)
C11	0.0285 (9)	0.0245 (8)	0.0248 (8)	−0.0082 (7)	0.0018 (7)	−0.0041 (6)
C12	0.0281 (9)	0.0235 (8)	0.0166 (8)	−0.0031 (7)	0.0029 (7)	−0.0006 (6)
C13	0.0335 (10)	0.0211 (8)	0.0256 (8)	−0.0058 (7)	0.0031 (7)	−0.0016 (6)
C14	0.0411 (10)	0.0206 (8)	0.0285 (9)	0.0042 (7)	0.0036 (7)	0.0011 (6)
C15	0.0253 (9)	0.0254 (8)	0.0352 (9)	0.0032 (7)	0.0018 (7)	0.0013 (7)
C16	0.0262 (9)	0.0211 (8)	0.0300 (9)	−0.0035 (7)	0.0018 (7)	−0.0002 (6)
C17	0.0248 (9)	0.0210 (8)	0.0170 (7)	−0.0009 (6)	0.0027 (6)	0.0001 (6)
C18	0.0244 (8)	0.0203 (7)	0.0170 (7)	−0.0019 (6)	0.0026 (6)	0.0001 (6)

Geometric parameters (Å, º)

F1—C1	1.3645 (18)	C12—C13	1.410 (2)
O1—C9	1.2877 (18)	C13—C14	1.369 (2)
N1—N2	1.2942 (16)	C14—C15	1.400 (2)
N1—C4	1.4120 (19)	C15—C16	1.374 (2)
N2—C18	1.3591 (19)	C16—C17	1.405 (2)
N1—H1N	0.8600	C17—C18	1.453 (2)
C1—C2	1.374 (2)	C2—H2	0.9300
C1—C6	1.376 (2)	C3—H3	0.9300
C2—C3	1.390 (2)	C5—H5	0.9300
C3—C4	1.388 (2)	C6—H6	0.9300
C4—C5	1.393 (2)	C10—H10	0.9300
C5—C6	1.378 (2)	C11—H11	0.9300
C9—C10	1.440 (2)	C13—H13	0.9300
C9—C18	1.442 (2)	C14—H14	0.9300
C10—C11	1.354 (2)	C15—H15	0.9300
C11—C12	1.438 (2)	C16—H16	0.9300
C12—C17	1.418 (2)		
N2—N1—C4	119.71 (13)	C12—C17—C18	119.02 (14)
N1—N2—C18	117.17 (13)	C16—C17—C18	122.71 (13)
C4—N1—H1N	120.00	C12—C17—C16	118.27 (13)
N2—N1—H1N	120.00	C9—C18—C17	120.42 (13)
F1—C1—C6	118.49 (14)	N2—C18—C9	123.53 (13)
C2—C1—C6	123.03 (15)	N2—C18—C17	116.05 (13)
F1—C1—C2	118.48 (13)	C1—C2—H2	121.00
C1—C2—C3	118.09 (14)	C3—C2—H2	121.00
C2—C3—C4	119.87 (14)	C2—C3—H3	120.00
N1—C4—C3	116.76 (13)	C4—C3—H3	120.00
C3—C4—C5	120.60 (13)	C4—C5—H5	120.00
N1—C4—C5	122.63 (13)	C6—C5—H5	120.00
C4—C5—C6	119.57 (14)	C1—C6—H6	121.00
C1—C6—C5	118.83 (15)	C5—C6—H6	121.00
C10—C9—C18	117.79 (13)	C9—C10—H10	119.00
O1—C9—C10	119.99 (14)	C11—C10—H10	119.00
O1—C9—C18	122.22 (13)	C10—C11—H11	119.00

C9—C10—C11	121.52 (15)	C12—C11—H11	119.00
C10—C11—C12	122.15 (14)	C12—C13—H13	120.00
C11—C12—C17	119.09 (13)	C14—C13—H13	120.00
C13—C12—C17	119.85 (14)	C13—C14—H14	120.00
C11—C12—C13	121.06 (14)	C15—C14—H14	120.00
C12—C13—C14	120.48 (14)	C14—C15—H15	120.00
C13—C14—C15	119.75 (14)	C16—C15—H15	120.00
C14—C15—C16	120.96 (15)	C15—C16—H16	120.00
C15—C16—C17	120.67 (14)	C17—C16—H16	120.00

C4—N1—N2—C18	178.88 (12)	C10—C9—C18—C17	1.1 (2)
N2—N1—C4—C3	168.30 (13)	C9—C10—C11—C12	0.2 (2)
N2—N1—C4—C5	−12.3 (2)	C10—C11—C12—C13	179.58 (13)
N1—N2—C18—C9	−2.7 (2)	C10—C11—C12—C17	0.2 (2)
N1—N2—C18—C17	177.94 (12)	C11—C12—C13—C14	179.94 (15)
F1—C1—C2—C3	−178.87 (16)	C17—C12—C13—C14	−0.7 (2)
C6—C1—C2—C3	0.3 (3)	C11—C12—C17—C16	−179.48 (13)
F1—C1—C6—C5	178.93 (16)	C11—C12—C17—C18	−0.02 (19)
C2—C1—C6—C5	−0.3 (3)	C13—C12—C17—C16	1.2 (2)
C1—C2—C3—C4	−0.3 (3)	C13—C12—C17—C18	−179.37 (13)
C2—C3—C4—N1	179.71 (14)	C12—C13—C14—C15	−0.4 (2)
C2—C3—C4—C5	0.3 (2)	C13—C14—C15—C16	1.0 (2)
N1—C4—C5—C6	−179.62 (15)	C14—C15—C16—C17	−0.5 (2)
C3—C4—C5—C6	−0.2 (2)	C15—C16—C17—C12	−0.6 (2)
C4—C5—C6—C1	0.2 (3)	C15—C16—C17—C18	179.97 (14)
O1—C9—C10—C11	179.18 (13)	C12—C17—C18—N2	178.74 (13)
C18—C9—C10—C11	−0.9 (2)	C12—C17—C18—C9	−0.7 (2)
O1—C9—C18—N2	1.7 (2)	C16—C17—C18—N2	−1.8 (2)
O1—C9—C18—C17	−178.98 (13)	C16—C17—C18—C9	178.78 (13)
C10—C9—C18—N2	−178.25 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1	0.86	1.83	2.5342 (18)	138
C3—H3···O1^{i}	0.93	2.54	3.417 (2)	157

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