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(*E*)-1-(3-Formylphenyl)-2-(2-oxidonaphthalen-1-yl)diazen-1-ium

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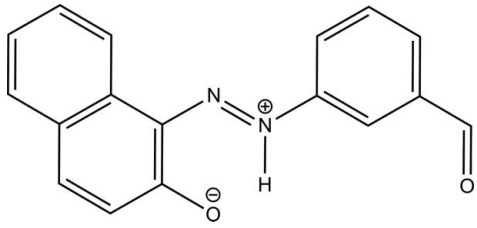
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.057; wR factor = 0.154; data-to-parameter ratio = 20.4.

In the title zwitterion, $C_{17}H_{12}N_2O_2$, the dihedral angle between the benzene ring and naphthalene ring system is 11.76 (7)° and an intramolecular N—H···O hydrogen bond exists. In the crystal, molecules are linked *via* pairs of C—H···O hydrogen bonds, forming inversion dimers.

Related literature

For general background to the use of azo compounds as dyes, pigments and advanced materials, see: Lee *et al.* (2004); Oueslati *et al.* (2004). For a related structure, see: Xu *et al.* (2010).



Experimental

Crystal data

$C_{17}H_{12}N_2O_2$
M_r = 276.29
Monoclinic, $P2_1/c$
a = 5.601 (4) Å
b = 7.780 (5) Å
c = 29.70 (2) Å
β = 94.624 (16)°
V = 1290.0 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.09 × 0.04 × 0.01 mm

Data collection

Nonius KappaCCD diffractometer
16470 measured reflections
3964 independent reflections
2155 reflections with $I > 2\sigma(I)$
R_{int} = 0.078

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.154
S = 1.01
3963 reflections
194 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.97 (3)	1.83 (3)	2.577 (3)	133 (3)
C6—H6···O1^{i}	0.93	2.41	3.327 (4)	168

Symmetry code: (i) $-x+2, -y+1, -z$.

Data collection: *KappaCCD Server Software* (Nonius, 1999); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; 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, 2012); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5735).

References

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supporting information

Acta Cryst. (2013). E**69**, o1498 [doi:10.1107/S1600536813024112]

(*E*)-1-(3-Formylphenyl)-2-(2-oxidonaphthalen-1-yl)diazen-1-ium

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S1. Comment

Azo compounds represent the dominant class of synthetic colourant employed in the textile, printing, agrochemical and pharmaceutical industries (Lee *et al.*, 2004); Oueslati *et al.*, 2004). As a result of the presence of the stable chromophoric azo group (N=N) which is capable of linking different aromatic systems with electron-donating and/or electron-withdrawing groups, dyes can be designed to resist chemical or photochemical degradation processes.

The molecular structure of (I) and the atom-numbering scheme are shown in Figure 1. Two aromatic rings A (C1—C6) and B (C7—C16) show a little deviation from planarity with a dihedral angle of 11.76 °. Intramolecular hydrogen bonds are formed between the phenol hydroxyl groups and the nearest N atom in the 3-aminobenzaldehyde groups [N—H—O = 2.577 (3)], similar to that reported previously (Xu *et al.*, 2010).

S2. Experimental

Treatment of 3-aminobenzaldehyde (0.02 mol) in 6 ml of 12*M* HCl and $NaNO_2$ (0.0214 mol) in 8 ml of H_2O for 30 min. To the obtained solution, was added dropwise a solution of naphthalen-2-ol, and the resulting brown precipitates were filtrated and washed with water, and dried in a desiccator for several days. Single crystals of I were obtained by slow evaporation from a pentane.

S3. Refinement

H1 atom was located in a difference Fourier map and refined isotropically. Other H atoms were positioned geometrically with C—H = 0.93 Å and refined in ridding mode with U_{iso}(H) = 1.2U_{eq}(C).

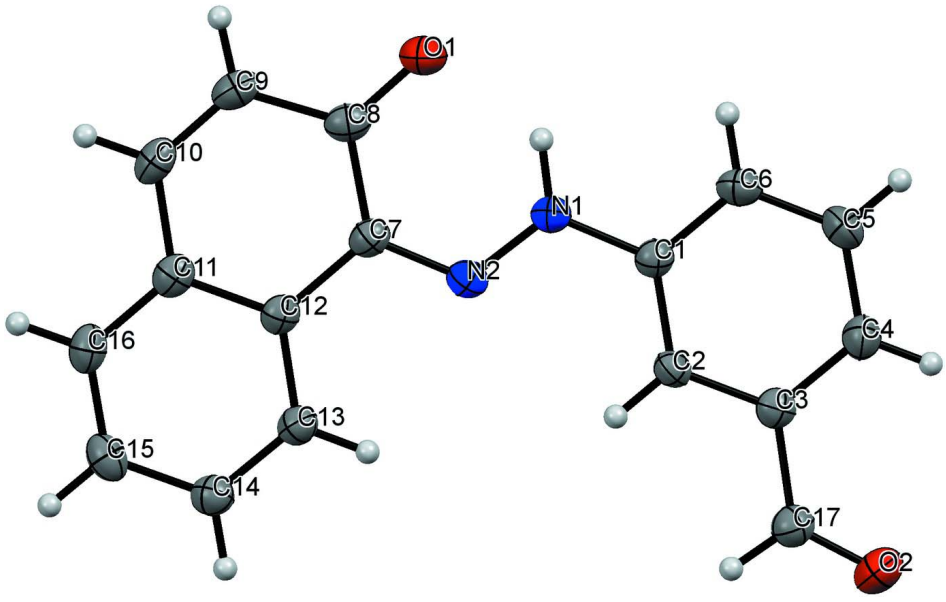

Figure 1

The molecular structure of the title molecule with the atom-numbering scheme. Hydrogen atoms is shown as a small spheres.

(*E*)-1-(3-Formylphenyl)-2-(2-oxidonaphthalen-1-yl)diazen-1-ium

Crystal data

$C_{17}H_{12}N_2O_2$
$M_r = 276.29$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.601$ (4) Å
$b = 7.780$ (5) Å
$c = 29.70$ (2) Å
$\beta = 94.624$ (16)°
$V = 1290.0$ (15) Å^3
$Z = 4$
$F(000) = 576$
$D_x = 1.423$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3964 reflections
$\theta = 1.3$–30.7°
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Needle, red
0.09 × 0.04 × 0.01 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
CCD rotation images, thick slices scans
16470 measured reflections
3964 independent reflections
2155 reflections with $I > 2\sigma(I)$
$R_{int} = 0.078$
$\theta_{max} = 30.7°$, $\theta_{min} = 1.4°$
$h = -7\rightarrow7$
$k = -11\rightarrow11$
$l = -42\rightarrow42$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.154$
$S = 1.01$
3963 reflections
194 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

$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.0107P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.1128 (2)	0.36260 (19)	0.05566 (4)	0.0354 (4)
O2	−0.0805 (2)	0.98626 (19)	0.12237 (5)	0.0382 (4)
N1	0.7771 (3)	0.5614 (2)	0.07936 (5)	0.0262 (4)
N2	0.8540 (3)	0.53524 (19)	0.12186 (5)	0.0244 (3)
C1	0.5770 (3)	0.6695 (2)	0.06949 (6)	0.0236 (4)
C2	0.4368 (3)	0.7287 (2)	0.10308 (6)	0.0233 (4)
H2	0.4746	0.6980	0.1331	0.028*
C3	0.2409 (3)	0.8333 (2)	0.09152 (6)	0.0252 (4)
C4	0.1826 (4)	0.8796 (3)	0.04653 (6)	0.0311 (5)
H4	0.0514	0.9500	0.0388	0.037*
C5	0.3226 (4)	0.8194 (3)	0.01347 (7)	0.0339 (5)
H5	0.2836	0.8488	−0.0166	0.041*
C6	0.5206 (4)	0.7156 (3)	0.02464 (6)	0.0307 (5)
H6	0.6147	0.6772	0.0023	0.037*
C7	1.0448 (3)	0.4360 (2)	0.13145 (6)	0.0244 (4)
C8	1.1796 (3)	0.3516 (2)	0.09708 (6)	0.0275 (4)
C9	1.3961 (3)	0.2599 (2)	0.11294 (7)	0.0299 (4)
H9	1.4850	0.2050	0.0921	0.036*
C10	1.4711 (3)	0.2523 (2)	0.15691 (7)	0.0289 (4)
H10	1.6132	0.1947	0.1654	0.035*
C11	1.3401 (3)	0.3301 (2)	0.19198 (6)	0.0260 (4)
C12	1.1257 (3)	0.4201 (2)	0.17941 (6)	0.0231 (4)
C13	0.9988 (3)	0.4950 (2)	0.21333 (6)	0.0262 (4)
H13	0.8574	0.5543	0.2054	0.031*
C14	1.0815 (3)	0.4817 (2)	0.25807 (6)	0.0291 (4)
H14	0.9957	0.5322	0.2801	0.035*
C15	1.2930 (4)	0.3929 (2)	0.27070 (7)	0.0306 (5)
H15	1.3478	0.3842	0.3010	0.037*
C16	1.4203 (3)	0.3179 (2)	0.23791 (6)	0.0289 (4)
H16	1.5610	0.2586	0.2464	0.035*

C17	0.0939 (4)	0.8931 (2)	0.12780 (7)	0.0299 (4)
H17	0.1386	0.8564	0.1571	0.036*
H1	0.862 (5)	0.511 (4)	0.0554 (10)	0.079 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0355 (8)	0.0430 (8)	0.0283 (8)	0.0046 (7)	0.0063 (6)	−0.0055 (6)
O2	0.0316 (8)	0.0381 (8)	0.0459 (9)	0.0057 (7)	0.0096 (7)	−0.0013 (7)
N1	0.0251 (8)	0.0315 (9)	0.0222 (8)	0.0016 (7)	0.0040 (7)	0.0001 (7)
N2	0.0250 (8)	0.0244 (8)	0.0240 (8)	−0.0036 (6)	0.0036 (6)	0.0014 (6)
C1	0.0221 (9)	0.0239 (9)	0.0250 (9)	−0.0017 (7)	0.0026 (7)	0.0012 (7)
C2	0.0228 (9)	0.0274 (9)	0.0197 (9)	−0.0023 (7)	0.0005 (7)	0.0001 (7)
C3	0.0236 (9)	0.0261 (9)	0.0261 (10)	−0.0037 (8)	0.0020 (7)	−0.0011 (8)
C4	0.0278 (10)	0.0339 (11)	0.0312 (11)	0.0044 (8)	−0.0003 (8)	0.0035 (8)
C5	0.0372 (12)	0.0425 (12)	0.0217 (9)	0.0040 (9)	0.0002 (8)	0.0050 (9)
C6	0.0325 (11)	0.0360 (11)	0.0246 (10)	0.0001 (9)	0.0079 (8)	0.0002 (8)
C7	0.0225 (9)	0.0224 (9)	0.0289 (10)	−0.0012 (7)	0.0048 (8)	0.0007 (7)
C8	0.0281 (10)	0.0258 (10)	0.0295 (10)	−0.0039 (8)	0.0081 (8)	−0.0015 (8)
C9	0.0253 (10)	0.0283 (10)	0.0374 (12)	0.0005 (8)	0.0104 (8)	−0.0037 (8)
C10	0.0210 (10)	0.0240 (9)	0.0422 (12)	0.0018 (8)	0.0055 (8)	0.0026 (8)
C11	0.0223 (9)	0.0221 (9)	0.0339 (10)	−0.0032 (7)	0.0037 (8)	0.0015 (8)
C12	0.0203 (9)	0.0223 (9)	0.0270 (10)	−0.0033 (7)	0.0029 (7)	0.0018 (7)
C13	0.0254 (9)	0.0252 (9)	0.0284 (10)	0.0016 (8)	0.0056 (8)	0.0014 (8)
C14	0.0327 (11)	0.0278 (10)	0.0272 (10)	0.0004 (8)	0.0049 (8)	0.0004 (8)
C15	0.0368 (11)	0.0270 (10)	0.0271 (10)	−0.0039 (8)	−0.0035 (9)	0.0036 (8)
C16	0.0248 (10)	0.0250 (10)	0.0362 (11)	−0.0001 (8)	−0.0021 (8)	0.0044 (8)
C17	0.0293 (10)	0.0297 (10)	0.0310 (11)	0.0003 (8)	0.0040 (8)	−0.0023 (8)

Geometric parameters (Å, º)

O1—C8	1.260 (2)	C7—C8	1.472 (3)
O2—C17	1.217 (2)	C8—C9	1.453 (3)
N1—N2	1.316 (2)	C9—C10	1.340 (3)
N1—C1	1.413 (2)	C9—H9	0.9300
N1—H1	0.97 (3)	C10—C11	1.454 (3)
N2—C7	1.331 (2)	C10—H10	0.9300
C1—C6	1.391 (3)	C11—C16	1.405 (3)
C1—C2	1.397 (3)	C11—C12	1.414 (3)
C2—C3	1.387 (3)	C12—C13	1.405 (3)
C2—H2	0.9300	C13—C14	1.375 (3)
C3—C4	1.397 (3)	C13—H13	0.9300
C3—C17	1.483 (3)	C14—C15	1.396 (3)
C4—C5	1.387 (3)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.382 (3)
C5—C6	1.390 (3)	C15—H15	0.9300
C5—H5	0.9300	C16—H16	0.9300
C6—H6	0.9300	C17—H17	0.9300

C7—C12	1.465 (3)		
N2—N1—C1	118.93 (16)	C10—C9—C8	121.69 (18)
N2—N1—H1	119.8 (17)	C10—C9—H9	119.2
C1—N1—H1	121.2 (17)	C8—C9—H9	119.2
N1—N2—C7	119.34 (16)	C9—C10—C11	122.90 (18)
C6—C1—C2	120.10 (17)	C9—C10—H10	118.6
C6—C1—N1	117.88 (17)	C11—C10—H10	118.6
C2—C1—N1	122.02 (17)	C16—C11—C12	119.23 (17)
C3—C2—C1	119.72 (17)	C16—C11—C10	121.81 (18)
C3—C2—H2	120.1	C12—C11—C10	118.96 (18)
C1—C2—H2	120.1	C13—C12—C11	118.94 (17)
C2—C3—C4	120.49 (17)	C13—C12—C7	121.84 (17)
C2—C3—C17	118.60 (17)	C11—C12—C7	119.20 (17)
C4—C3—C17	120.91 (18)	C14—C13—C12	120.71 (18)
C5—C4—C3	119.22 (19)	C14—C13—H13	119.6
C5—C4—H4	120.4	C12—C13—H13	119.6
C3—C4—H4	120.4	C13—C14—C15	120.62 (18)
C4—C5—C6	120.87 (18)	C13—C14—H14	119.7
C4—C5—H5	119.6	C15—C14—H14	119.7
C6—C5—H5	119.6	C16—C15—C14	119.64 (18)
C5—C6—C1	119.59 (18)	C16—C15—H15	120.2
C5—C6—H6	120.2	C14—C15—H15	120.2
C1—C6—H6	120.2	C15—C16—C11	120.86 (18)
N2—C7—C12	115.93 (16)	C15—C16—H16	119.6
N2—C7—C8	123.94 (17)	C11—C16—H16	119.6
C12—C7—C8	120.07 (17)	O2—C17—C3	125.28 (19)
O1—C8—C9	121.63 (17)	O2—C17—H17	117.4
O1—C8—C7	121.23 (18)	C3—C17—H17	117.4
C9—C8—C7	117.11 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.97 (3)	1.83 (3)	2.577 (3)	133 (3)
C6—H6···O1^{i}	0.93	2.41	3.327 (4)	168

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.