Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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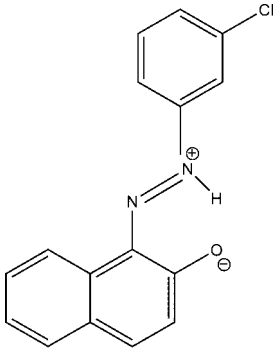
Received 15 May 2013; accepted 30 May 2013

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.059; wR factor = 0.185; data-to-parameter ratio = 14.1.

The title zwitterion,, $C_{16}H_{11}ClN_2O$, is approximately planar, the dihedral angle between the benzene ring and naphthalene ring system is 1.55 (13)°; an intramolecular N—H···O hydrogen bond stabilizes the planar conformation. In the crystal, π–π stacking between the benzene ring and the naphthalene ring system of adjacent molecules links the molecules into supramolecular chains running along the b axis, the centroid–centroid distance being 3.765 (2) Å.

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). Many azo compounds have been synthesized by diazotization and diazo-coupling reactions; for information, see: Wang *et al.* (2003). For a related structure, see: Elmali *et al.* (2001).



Experimental

Crystal data

$C_{16}H_{11}ClN_2O$
M_r = 282.72
Monoclinic, $P2_1/c$
a = 16.340 (2) Å
b = 5.7665 (4) Å
c = 15.632 (2) Å
β = 113.604 (4)°
V = 1349.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 293 K
0.09 × 0.04 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
4488 measured reflections
2418 independent reflections
1289 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.185
S = 1.01
2418 reflections
171 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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	1.82	2.564 (4)	135

Data collection: *KappaCCD Reference Manual* (Nonius, 1998); 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*.

We are grateful to Mr L. Ouahab (University of Rennes, France) for his collaboration in the recording and interpretation of XRD data and express our gratitude for the valuable assistance he has provided throughout the realisation of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5708).

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supporting information

Acta Cryst. (2013). E**69**, o1021 [https://doi.org/10.1107/S1600536813014931]

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

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S1. 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 pigments 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 was obtained through the diazotization of 3-chloroaniline followed by a coupling reaction with 2-naphthol.

This compound, which has a non-planar molecular structure, contains two aromatic rings linked through a imine group. The dihedral angle between the two aromatic rings C1—C6 and C7—C16 is 1.55 (13)°. Intramolecular N—H···O hydrogen bond is observed in the molecular structure, similar to that in a reported structure (Elmali *et al.*, 2001). In the crystal structure, molecules are linked through π-π stacking between benzene ring and naphthalene ring system of adjacent molecules, the centroid-centroid distance between C1-ring and C7^{i}-ring being 3.765 (2) Å (symmetry code: i = x, -1+y, z).

S2. Experimental

The title compound was obtained through the diazotization of 3-chloroaniline followed by a coupling reaction with 2-naphthol. Crystals suitable for X-ray analysis were obtained by slow evaporation of a pentane solution.

S3. Refinement

H atoms were positioned geometrically with C—H = 0.93 and N—H = 0.94 Å, and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

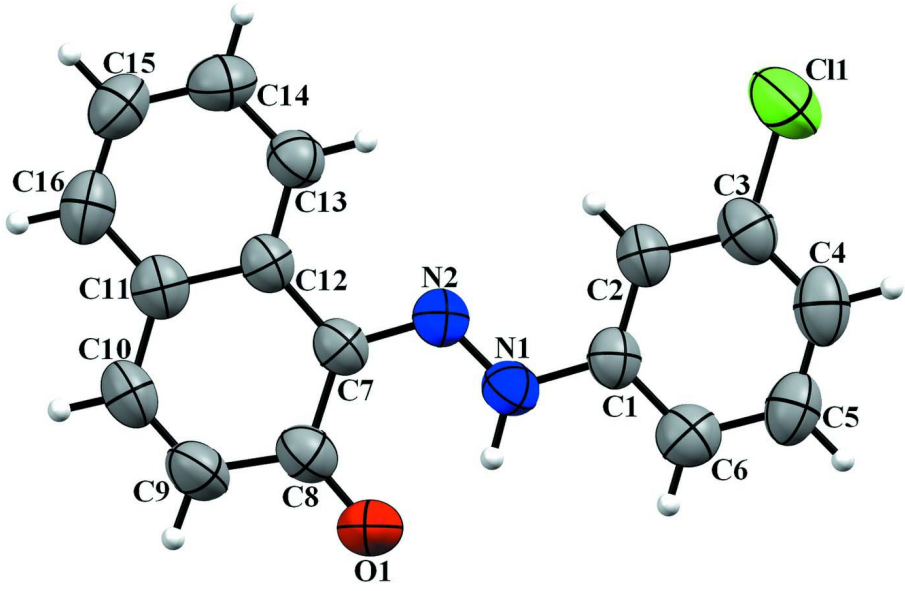

Figure 1

The molecular structure.

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

Crystal data

$C_{16}H_{11}ClN_2O$
$M_r = 282.72$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 16.340$ (2) Å
$b = 5.7665$ (4) Å
$c = 15.632$ (2) Å
$\beta = 113.604$ (4)°
$V = 1349.7$ (3) Å^3
$Z = 4$
$F(000) = 584$
$D_x = 1.391$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2548 reflections
$\theta = 2.9$–25.4°
$\mu = 0.28$ mm^{-1}
$T = 293$ K
Needle, red
0.09 × 0.04 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Horizonally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
CCD rotation images, thick slices scans
4488 measured reflections
2418 independent reflections
1289 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.3°$, $\theta_{min} = 3.1°$
$h = -19\rightarrow19$
$k = -6\rightarrow6$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.185$
$S = 1.01$
2418 reflections
171 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
$w = 1/[\sigma^2(F_o^2) + (0.0928P)^2 + 0.1732P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ 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 e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.06364 (8)	−0.5972 (2)	0.37478 (9)	0.1078 (5)
O1	0.46478 (16)	0.1141 (4)	0.38441 (18)	0.0786 (9)
N1	0.33259 (17)	−0.1220 (4)	0.38634 (18)	0.0572 (9)
N2	0.27805 (17)	0.0115 (4)	0.32242 (17)	0.0528 (8)
C1	0.2977 (2)	−0.3084 (5)	0.4184 (2)	0.0535 (10)
C2	0.2070 (2)	−0.3500 (5)	0.3853 (2)	0.0583 (11)
C3	0.1771 (2)	−0.5415 (6)	0.4175 (2)	0.0667 (12)
C4	0.2351 (3)	−0.6891 (6)	0.4821 (3)	0.0746 (14)
C5	0.3258 (3)	−0.6464 (6)	0.5165 (2)	0.0708 (14)
C6	0.3578 (2)	−0.4547 (6)	0.4852 (2)	0.0666 (12)
C7	0.3117 (2)	0.1901 (5)	0.2907 (2)	0.0523 (11)
C8	0.4066 (2)	0.2395 (5)	0.3238 (2)	0.0613 (11)
C9	0.4306 (2)	0.4390 (6)	0.2841 (3)	0.0714 (14)
C10	0.3705 (3)	0.5765 (6)	0.2221 (3)	0.0670 (12)
C11	0.2759 (2)	0.5349 (5)	0.1888 (2)	0.0572 (11)
C12	0.2463 (2)	0.3361 (5)	0.2220 (2)	0.0504 (10)
C13	0.1542 (2)	0.2970 (5)	0.1879 (2)	0.0618 (11)
C14	0.0948 (2)	0.4492 (6)	0.1263 (3)	0.0730 (12)
C15	0.1241 (3)	0.6417 (6)	0.0963 (2)	0.0698 (14)
C16	0.2134 (3)	0.6844 (5)	0.1264 (2)	0.0684 (13)
H1	0.39440	−0.10220	0.40590	0.0690*
H2	0.16670	−0.25050	0.34200	0.0700*
H4	0.21350	−0.81740	0.50270	0.0900*
H5	0.36550	−0.74560	0.56060	0.0850*
H6	0.41880	−0.42450	0.50860	0.0800*
H9	0.49090	0.47380	0.30250	0.0860*
H10	0.39040	0.70430	0.19950	0.0800*
H13	0.13290	0.16620	0.20720	0.0740*
H14	0.03380	0.42060	0.10480	0.0870*
H15	0.08320	0.74400	0.05520	0.0840*
H16	0.23270	0.81510	0.10510	0.0820*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0856 (8)	0.1168 (9)	0.1281 (10)	−0.0275 (6)	0.0501 (7)	0.0075 (7)
O1	0.0545 (15)	0.0780 (15)	0.0954 (19)	0.0021 (12)	0.0218 (14)	0.0107 (14)
N1	0.0531 (16)	0.0556 (14)	0.0611 (17)	−0.0055 (13)	0.0212 (14)	−0.0046 (14)
N2	0.0587 (16)	0.0505 (13)	0.0489 (15)	−0.0023 (12)	0.0213 (13)	−0.0068 (12)
C1	0.066 (2)	0.0448 (16)	0.0501 (18)	−0.0040 (14)	0.0237 (17)	−0.0070 (14)
C2	0.067 (2)	0.0518 (17)	0.059 (2)	−0.0067 (16)	0.0284 (17)	−0.0001 (16)
C3	0.076 (2)	0.068 (2)	0.063 (2)	−0.0122 (18)	0.035 (2)	−0.0072 (18)
C4	0.111 (3)	0.056 (2)	0.065 (2)	−0.010 (2)	0.044 (2)	−0.0048 (18)
C5	0.096 (3)	0.058 (2)	0.056 (2)	0.0043 (19)	0.028 (2)	0.0039 (17)
C6	0.072 (2)	0.066 (2)	0.058 (2)	−0.0013 (17)	0.0222 (18)	−0.0094 (17)
C7	0.055 (2)	0.0517 (17)	0.0529 (18)	−0.0054 (14)	0.0244 (16)	−0.0074 (15)
C8	0.059 (2)	0.0605 (19)	0.067 (2)	−0.0076 (17)	0.0281 (18)	−0.0088 (17)
C9	0.058 (2)	0.077 (2)	0.086 (3)	−0.0100 (19)	0.036 (2)	−0.003 (2)
C10	0.076 (2)	0.063 (2)	0.071 (2)	−0.0154 (18)	0.039 (2)	−0.0017 (17)
C11	0.070 (2)	0.0540 (17)	0.0536 (19)	−0.0028 (16)	0.0310 (17)	−0.0088 (15)
C12	0.0576 (19)	0.0468 (16)	0.0502 (18)	−0.0044 (14)	0.0251 (15)	−0.0082 (14)
C13	0.060 (2)	0.0612 (19)	0.062 (2)	−0.0075 (16)	0.0220 (18)	−0.0024 (17)
C14	0.058 (2)	0.082 (2)	0.069 (2)	0.0026 (19)	0.0149 (18)	−0.003 (2)
C15	0.078 (3)	0.063 (2)	0.059 (2)	0.0111 (19)	0.0177 (19)	0.0035 (17)
C16	0.097 (3)	0.0522 (19)	0.057 (2)	0.0012 (18)	0.032 (2)	0.0015 (17)

Geometric parameters (Å, º)

Cl1—C3	1.731 (4)	C11—C16	1.393 (5)
O1—C8	1.266 (4)	C11—C12	1.421 (4)
N1—N2	1.293 (4)	C12—C13	1.399 (5)
N1—C1	1.400 (4)	C13—C14	1.375 (5)
N2—C7	1.352 (4)	C14—C15	1.364 (5)
N1—H1	0.9400	C15—C16	1.364 (7)
C1—C2	1.381 (5)	C2—H2	0.9300
C1—C6	1.395 (4)	C4—H4	0.9300
C2—C3	1.382 (5)	C5—H5	0.9300
C3—C4	1.370 (5)	C6—H6	0.9300
C4—C5	1.381 (7)	C9—H9	0.9300
C5—C6	1.393 (5)	C10—H10	0.9300
C7—C8	1.453 (5)	C13—H13	0.9300
C7—C12	1.444 (4)	C14—H14	0.9300
C8—C9	1.434 (5)	C15—H15	0.9300
C9—C10	1.331 (6)	C16—H16	0.9300
C10—C11	1.440 (6)		
N2—N1—C1	118.7 (3)	C7—C12—C11	118.9 (3)
N1—N2—C7	118.8 (3)	C7—C12—C13	123.5 (3)
C1—N1—H1	121.00	C12—C13—C14	120.9 (3)
N2—N1—H1	120.00	C13—C14—C15	120.9 (4)

N1—C1—C6	117.8 (3)	C14—C15—C16	120.2 (3)
C2—C1—C6	120.2 (3)	C11—C16—C15	120.9 (3)
N1—C1—C2	121.9 (3)	C1—C2—H2	120.00
C1—C2—C3	119.0 (3)	C3—C2—H2	121.00
Cl1—C3—C4	119.2 (3)	C3—C4—H4	120.00
Cl1—C3—C2	119.2 (3)	C5—C4—H4	120.00
C2—C3—C4	121.6 (3)	C4—C5—H5	120.00
C3—C4—C5	119.6 (4)	C6—C5—H5	120.00
C4—C5—C6	120.0 (3)	C1—C6—H6	120.00
C1—C6—C5	119.5 (3)	C5—C6—H6	120.00
C8—C7—C12	121.1 (3)	C8—C9—H9	119.00
N2—C7—C8	123.5 (3)	C10—C9—H9	119.00
N2—C7—C12	115.4 (3)	C9—C10—H10	119.00
C7—C8—C9	116.2 (3)	C11—C10—H10	119.00
O1—C8—C9	121.9 (3)	C12—C13—H13	119.00
O1—C8—C7	121.9 (3)	C14—C13—H13	120.00
C8—C9—C10	122.9 (4)	C13—C14—H14	120.00
C9—C10—C11	122.4 (4)	C15—C14—H14	120.00
C12—C11—C16	119.6 (3)	C14—C15—H15	120.00
C10—C11—C12	118.4 (3)	C16—C15—H15	120.00
C10—C11—C16	122.0 (3)	C11—C16—H16	120.00
C11—C12—C13	117.6 (3)	C15—C16—H16	120.00

C1—N1—N2—C7	−179.3 (3)	N2—C7—C12—C13	−1.3 (4)
N2—N1—C1—C2	−1.5 (4)	C8—C7—C12—C11	−1.9 (4)
N2—N1—C1—C6	178.0 (3)	C8—C7—C12—C13	−179.8 (3)
N1—N2—C7—C8	0.8 (4)	O1—C8—C9—C10	−178.3 (4)
N1—N2—C7—C12	−177.7 (3)	C7—C8—C9—C10	1.5 (5)
N1—C1—C2—C3	177.8 (3)	C8—C9—C10—C11	−0.7 (6)
C6—C1—C2—C3	−1.7 (5)	C9—C10—C11—C12	−1.6 (6)
N1—C1—C6—C5	−177.9 (3)	C9—C10—C11—C16	177.7 (4)
C2—C1—C6—C5	1.6 (5)	C10—C11—C12—C7	2.8 (4)
C1—C2—C3—Cl1	−178.9 (2)	C10—C11—C12—C13	−179.2 (3)
C1—C2—C3—C4	0.8 (5)	C16—C11—C12—C7	−176.5 (3)
Cl1—C3—C4—C5	179.9 (3)	C16—C11—C12—C13	1.5 (4)
C2—C3—C4—C5	0.2 (6)	C10—C11—C16—C15	−179.6 (3)
C3—C4—C5—C6	−0.3 (6)	C12—C11—C16—C15	−0.4 (5)
C4—C5—C6—C1	−0.7 (5)	C7—C12—C13—C14	176.4 (3)
N2—C7—C8—O1	1.1 (5)	C11—C12—C13—C14	−1.6 (5)
N2—C7—C8—C9	−178.7 (3)	C12—C13—C14—C15	0.4 (5)
C12—C7—C8—O1	179.6 (3)	C13—C14—C15—C16	0.8 (6)
C12—C7—C8—C9	−0.2 (4)	C14—C15—C16—C11	−0.8 (5)
N2—C7—C12—C11	176.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.94	1.82	2.564 (4)	135