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(*E*)-1-(3-Chlorophenyl)-2-(2-oxidonaphthalen-1-yl)diazenium

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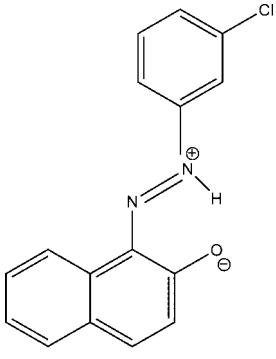
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.059; wR factor = 0.185; data-to-parameter ratio = 14.1.

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*.

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

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