Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,1′-[(1*E*,11*E*)-5,8-Dioxa-2,11-diazoniadodeca-1,11-diene-1,12-diyl]dinaphthalen-2-olate

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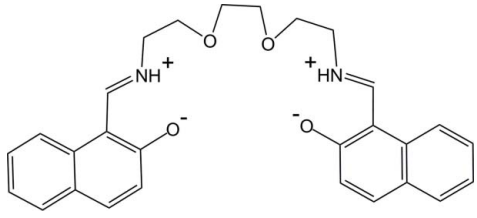
Received 22 March 2011; accepted 1 April 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.068; wR factor = 0.224; data-to-parameter ratio = 13.3.

The title compound, $C_{28}H_{28}N_2O_4$, crystallizes in a zwitterionic form with deprotonated naphthol hydroxy groups and protonated imine N atoms. The asymmetric unit contains one half-molecule located on a twofold rotation axis. Intramolecular N—H···O hydrogen bonds occur and the two bicyclic ring systems form a dihedral angle of 64.2 (1)°. In the crystal, weak intermolecular C—H···O hydrogen bonds link the molecules into layers parallel to the *bc* plane.

Related literature

For applications of Schiff bases in coordination chemistry, see: Osowle (2008). For related structures, see: Etemadi *et al.* (2004); Liu *et al.* (2010); Farag *et al.* (2010; 2011).



Experimental

Crystal data

$C_{28}H_{28}N_2O_4$
M_r = 456.52
Orthorhombic, *Pcca*
a = 44.704 (4) Å
b = 6.3576 (6) Å
c = 8.2074 (9) Å
V = 2332.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.50 × 0.37 × 0.11 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.958, T_{max} = 0.991
9099 measured reflections
2060 independent reflections
1162 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.224
S = 1.00
2060 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	1.85	2.542 (5)	136
C14—H14B···O2^{i}	0.97	2.58	3.382 (5)	141
C12—H12B···O1^{ii}	0.97	2.50	3.257 (5)	134

Symmetry codes: (i) $x, -y+1, z+\frac{1}{2}$; (ii) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5066).

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supplementary materials

Acta Cryst. (2011). E**67**, o1074 [**doi:10.1107/S1600536811012219**]

1,1'-[(1*E*,11*E*)-5,8-Dioxa-2,11-diazoniadodeca-1,11-diene-1,12-diyl]dinaphthalen-2-olate

Y. Liu, K. Liu, Z. Cao and M. Niu

Comment

Schiff bases have various applications in coordination chemistry (Osowle, 2008). Herewith we present the title compound (I), which is a new crowned Schiff base.

In (I) (Fig. 1), all bond lengths and angles are usual and comparable with those observed in the related compounds (Etemadi *et al.*, 2004; Liu *et al.*, 2010; Farag *et al.*, 2010, 2011). Each molecule is situated on a twofold rotational axis. Intramolecular N—H···O hydrogen bonds (Table 1) influence the molecular conformation - two bicycles form a dihedral angle of 64.2 (1)°. In the crystal structure, weak intermolecular C—H···O hydrogen bonds (Table 1) link molecules into layers parallel to *bc* plane.

Experimental

The title compound was synthesized by adding drop-wise a solution of 3,6-dioxa-1,8-diaminooctane (1.48 g,10 mmol) in absolute methanol (10 mL) to a methanol solution (20 mL) of 2-hydroxy-1-naphthaldehyde (3.4438 g,20 mmol) under stirring at room temperature. The resultant reaction mixture was then refluxed for 5 h, cooled and concentrated under reduced pressure, and then the residue was retained at -268 K for overnight. The bright yellow crystal which suitable for X-ray analysis was formed, filtered and dried under reduced pressure.Yield:82%. Analysis found: C 73.07, H 6.06, N 6.51%; calculated for $C_{28}H_{28}N_2O_4$ (Mr=456.54): C 73.66, H 6.18, N 6.14%.

Refinement

C-bound H atoms were geometrically positioned [C—H 0.93–0.97 Å]. Atom H1A was located on a difference map, but placed in idealized position [N—H 0.86 Å]. All H atoms were refined as riding atoms, with U_{iso}(H) = 1.2–1.5 U_{iso} of the parent atom.

Figures

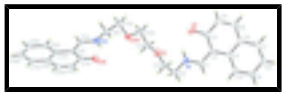


Fig. 1. The molecular structure of (I) showing the atomic labels and 30% probability displacement ellipsoids. Symmetry code: (A) -*x* + 1/2,-*y* + 1,*z*.

1,1'-[(1*E*,11*E*)-5,8-Dioxa-2,11-diazoniadodeca-1,11-diene-\ 1,12-diyl]dinaphthalen-2-olate

Crystal data

$C_{28}H_{28}N_2O_4$	$F(000) = 968$
$M_r = 456.52$	$D_x = 1.300$ Mg m^{-3}
Orthorhombic, *Pcca*	Mo *K*α radiation, λ = 0.71073 Å

Hall symbol: -P 2a 2ac	Cell parameters from 1398 reflections
a = 44.704 (4) Å	θ = 2.7–22.6°
b = 6.3576 (6) Å	μ = 0.09 mm^{-1}
c = 8.2074 (9) Å	T = 298 K
V = 2332.6 (4) Å^3	Block, yellow
Z = 4	0.50 × 0.37 × 0.11 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2060 independent reflections
Radiation source: fine-focus sealed tube	1162 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.081
phi and ω scans	θ_{max} = 25.0°, θ_{min} = 1.8°
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	h = −53→28
T_{min} = 0.958, T_{max} = 0.991	k = −7→7
9099 measured reflections	l = −9→9

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.068	H-atom parameters constrained
$wR(F^2)$ = 0.224	$w = 1/[\sigma^2(F_o^2) + (0.088P)^2 + 3.8548P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
2060 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
155 parameters	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
0 restraints	Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0055 (16)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.16369 (7)	0.4462 (5)	0.0795 (4)	0.0479 (10)
H1A	0.1720	0.5537	0.1239	0.058*
C2	0.11853 (8)	0.6454 (6)	0.0728 (5)	0.0370 (9)
O1	0.15974 (7)	0.8123 (5)	0.2021 (4)	0.0628 (10)
O2	0.22075 (6)	0.4082 (5)	0.2116 (4)	0.0541 (9)
C11	0.08741 (8)	0.6581 (6)	0.0253 (5)	0.0388 (10)
C1	0.13580 (8)	0.4646 (6)	0.0400 (5)	0.0402 (10)
H1	0.1266	0.3525	−0.0129	0.048*
C6	0.07056 (9)	0.8373 (6)	0.0703 (5)	0.0464 (11)
C3	0.13216 (10)	0.8124 (6)	0.1618 (5)	0.0463 (11)

C10	0.07267 (8)	0.5045 (7)	−0.0672 (5)	0.0469 (11)
H10	0.0832	0.3861	−0.1007	0.056*
C12	0.18209 (9)	0.2620 (7)	0.0560 (6)	0.0505 (12)
H12A	0.1941	0.2793	−0.0415	0.061*
H12B	0.1694	0.1397	0.0410	0.061*
C4	0.11373 (10)	0.9880 (7)	0.2060 (6)	0.0557 (12)
H4	0.1220	1.0978	0.2657	0.067*
C5	0.08502 (10)	0.9976 (7)	0.1636 (5)	0.0550 (12)
H5	0.0739	1.1138	0.1962	0.066*
C8	0.02674 (10)	0.6990 (9)	−0.0632 (6)	0.0650 (14)
H8	0.0067	0.7120	−0.0922	0.078*
C7	0.04054 (10)	0.8504 (8)	0.0252 (6)	0.0572 (13)
H7	0.0296	0.9677	0.0571	0.069*
C9	0.04327 (9)	0.5238 (8)	−0.1096 (6)	0.0553 (12)
H9	0.0342	0.4182	−0.1703	0.066*
C13	0.20210 (9)	0.2282 (7)	0.1994 (6)	0.0566 (13)
H13A	0.1903	0.2115	0.2979	0.068*
H13B	0.2141	0.1027	0.1840	0.068*
C14	0.24105 (8)	0.4015 (7)	0.3430 (5)	0.0507 (12)
H14A	0.2542	0.2808	0.3319	0.061*
H14B	0.2302	0.3884	0.4449	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0378 (17)	0.048 (2)	0.059 (2)	−0.0032 (15)	−0.0074 (17)	0.0003 (19)
C2	0.041 (2)	0.035 (2)	0.035 (2)	−0.0033 (17)	−0.0019 (18)	0.0031 (18)
O1	0.066 (2)	0.0485 (19)	0.074 (2)	−0.0125 (15)	−0.0256 (18)	0.0002 (17)
O2	0.0413 (15)	0.064 (2)	0.057 (2)	−0.0092 (14)	−0.0097 (14)	0.0128 (16)
C11	0.042 (2)	0.042 (2)	0.032 (2)	0.0007 (18)	0.0030 (18)	0.0051 (19)
C1	0.039 (2)	0.042 (2)	0.040 (2)	−0.0059 (17)	−0.0017 (19)	0.0059 (19)
C6	0.054 (2)	0.043 (2)	0.043 (3)	0.000 (2)	0.007 (2)	0.004 (2)
C3	0.059 (3)	0.037 (2)	0.043 (3)	−0.006 (2)	−0.005 (2)	0.004 (2)
C10	0.043 (2)	0.050 (2)	0.049 (3)	−0.003 (2)	−0.004 (2)	−0.003 (2)
C12	0.040 (2)	0.054 (3)	0.057 (3)	0.000 (2)	−0.003 (2)	−0.003 (2)
C4	0.081 (3)	0.041 (2)	0.046 (3)	−0.011 (3)	−0.004 (3)	−0.002 (2)
C5	0.074 (3)	0.043 (3)	0.049 (3)	0.006 (2)	0.006 (2)	0.001 (2)
C8	0.040 (2)	0.091 (4)	0.064 (3)	0.005 (3)	−0.001 (2)	0.001 (3)
C7	0.052 (3)	0.061 (3)	0.059 (3)	0.017 (2)	0.008 (2)	0.005 (3)
C9	0.045 (2)	0.068 (3)	0.053 (3)	−0.001 (2)	−0.006 (2)	−0.005 (3)
C13	0.047 (2)	0.054 (3)	0.069 (3)	0.000 (2)	−0.011 (2)	0.004 (3)
C14	0.044 (2)	0.067 (3)	0.042 (3)	0.004 (2)	−0.003 (2)	0.005 (2)

Geometric parameters (Å, °)

N1—C1	1.294 (4)	C12—C13	1.494 (6)
N1—C12	1.444 (5)	C12—H12A	0.9700
N1—H1A	0.8600	C12—H12B	0.9700
C2—C1	1.410 (5)	C4—C5	1.331 (6)

C2—C3	1.426 (5)	C4—H4	0.9300
C2—C11	1.447 (5)	C5—H5	0.9300
O1—C3	1.276 (5)	C8—C7	1.354 (7)
O2—C14	1.410 (5)	C8—C9	1.390 (6)
O2—C13	1.420 (5)	C8—H8	0.9300
C11—C10	1.402 (5)	C7—H7	0.9300
C11—C6	1.415 (5)	C9—H9	0.9300
C1—H1	0.9300	C13—H13A	0.9700
C6—C7	1.394 (6)	C13—H13B	0.9700
C6—C5	1.429 (6)	C14—C14^{i}	1.486 (8)
C3—C4	1.434 (6)	C14—H14A	0.9700
C10—C9	1.365 (5)	C14—H14B	0.9700
C10—H10	0.9300		
C1—N1—C12	126.1 (4)	C5—C4—C3	121.6 (4)
C1—N1—H1A	117.0	C5—C4—H4	119.2
C12—N1—H1A	117.0	C3—C4—H4	119.2
C1—C2—C3	118.1 (3)	C4—C5—C6	122.9 (4)
C1—C2—C11	121.4 (3)	C4—C5—H5	118.6
C3—C2—C11	120.5 (4)	C6—C5—H5	118.6
C14—O2—C13	114.1 (3)	C7—C8—C9	118.3 (4)
C10—C11—C6	116.9 (4)	C7—C8—H8	120.8
C10—C11—C2	124.0 (4)	C9—C8—H8	120.8
C6—C11—C2	119.1 (4)	C8—C7—C6	122.6 (4)
N1—C1—C2	123.6 (4)	C8—C7—H7	118.7
N1—C1—H1	118.2	C6—C7—H7	118.7
C2—C1—H1	118.2	C10—C9—C8	120.9 (5)
C7—C6—C11	119.4 (4)	C10—C9—H9	119.5
C7—C6—C5	122.3 (4)	C8—C9—H9	119.5
C11—C6—C5	118.2 (4)	O2—C13—C12	106.9 (4)
O1—C3—C2	123.1 (4)	O2—C13—H13A	110.3
O1—C3—C4	119.3 (4)	C12—C13—H13A	110.3
C2—C3—C4	117.6 (4)	O2—C13—H13B	110.3
C9—C10—C11	121.9 (4)	C12—C13—H13B	110.3
C9—C10—H10	119.1	H13A—C13—H13B	108.6
C11—C10—H10	119.1	O2—C14—C14^{i}	108.7 (3)
N1—C12—C13	110.7 (4)	O2—C14—H14A	109.9
N1—C12—H12A	109.5	C14^{i}—C14—H14A	109.9
C13—C12—H12A	109.5	O2—C14—H14B	109.9
N1—C12—H12B	109.5	C14^{i}—C14—H14B	109.9
C13—C12—H12B	109.5	H14A—C14—H14B	108.3
H12A—C12—H12B	108.1		
C1—C2—C11—C10	−5.6 (6)	C2—C11—C10—C9	−179.8 (4)
C3—C2—C11—C10	177.6 (4)	C1—N1—C12—C13	−140.1 (4)
C1—C2—C11—C6	175.9 (4)	O1—C3—C4—C5	178.5 (4)
C3—C2—C11—C6	−0.9 (6)	C2—C3—C4—C5	−1.1 (7)
C12—N1—C1—C2	177.0 (4)	C3—C4—C5—C6	−0.8 (7)
C3—C2—C1—N1	−3.4 (6)	C7—C6—C5—C4	−179.3 (5)
C11—C2—C1—N1	179.8 (4)	C11—C6—C5—C4	1.8 (7)

C10—C11—C6—C7	1.5 (6)	C9—C8—C7—C6	0.3 (7)
C2—C11—C6—C7	−179.9 (4)	C11—C6—C7—C8	−1.1 (7)
C10—C11—C6—C5	−179.5 (4)	C5—C6—C7—C8	180.0 (4)
C2—C11—C6—C5	−0.9 (6)	C11—C10—C9—C8	0.5 (7)
C1—C2—C3—O1	5.5 (6)	C7—C8—C9—C10	0.0 (7)
C11—C2—C3—O1	−177.7 (4)	C14—O2—C13—C12	179.6 (3)
C1—C2—C3—C4	−175.0 (4)	N1—C12—C13—O2	−61.2 (5)
C11—C2—C3—C4	1.8 (6)	C13—O2—C14—C14^{i}	−179.5 (4)
C6—C11—C10—C9	−1.3 (6)		

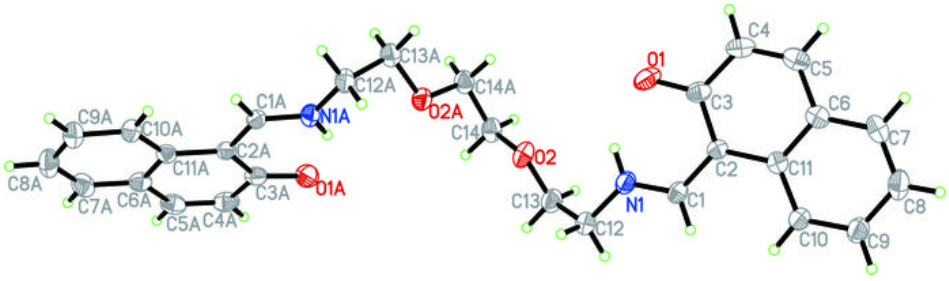
Symmetry codes: (i) −*x*+1/2, −*y*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1	0.86	1.85	2.542 (5)	136
C14—H14B···O2^{ii}	0.97	2.58	3.382 (5)	141
C12—H12B···O1^{iii}	0.97	2.50	3.257 (5)	134

Symmetry codes: (ii) *x*, −*y*+1, *z*+1/2; (iii) *x*, *y*−1, *z*.

Fig. 1


C4
O1
C5
C3
C6
C7
C2
C11
C1
N1
C8
C10
C9
C12
C13
O2
C14
C13A
C14A
O2A
C12A
N1A
C1A
C9A
C10A
C2A
C11A
C8A
C7A
C6A
C5A
C4A
C3A
O1A