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(*E*)-1-[(2-Hydroxy-1-naphthyl)methylideneamino]imidazolidine-2,4-dione

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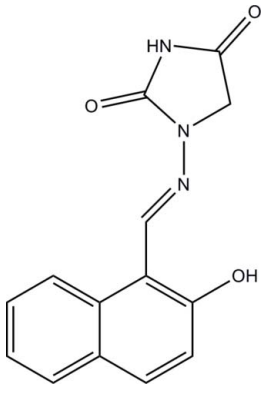
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.067; data-to-parameter ratio = 11.5.

The title compound, $C_{14}H_{11}N_3O_3$, adopts an *E* or *trans* configuration with respect to the C=N bond. In the molecule there is an intramolecular O—H···N hydrogen bond involving the hydroxy substituent at the 2-positon of the naphthalene ring and the adjacent methyleneamino N atom. The molecule is roughly planar, the dihedral angle between the naphthalene and imidazolidine-2,4-dione mean planes being 8.4 (1)°. In the crystal, pairs of N—H···O hydrogen bonds link molecules into inversion dimers. These dimers are futher linked *via* C—H···O interactions, forming a three-dimensional network.

Related literature

For the naphthalene group as a fluorophore, see: Li *et al.* (2010); Iijima *et al.* (2010). For a related structure, see: Xu *et al.* (2009). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{11}N_3O_3$
M_r = 269.26
Monoclinic, $P2_1/c$
a = 11.5122 (7) Å
b = 6.0233 (3) Å
c = 17.9955 (10) Å
β = 96.773 (5)°
V = 1239.13 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.40 × 0.30 × 0.30 mm

Data collection

Oxford Diffraction Gemini S Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.959, T_{max} = 0.969
4288 measured reflections
2136 independent reflections
1053 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.067
S = 0.72
2136 reflections
186 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3*N*···O1^{i}	0.890 (18)	1.962 (18)	2.851 (2)	177.9 (19)
O3—H4···N1	0.82	1.91	2.622 (2)	145
C6—H6···O2^{ii}	0.93	2.55	3.469 (2)	169
C14—H14*B*···O2^{ii}	0.97	2.36	3.038 (2)	127

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: SU2180).

References

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supporting information

Acta Cryst. (2010). E**66**, o1601 [doi:10.1107/S1600536810020118]

(*E*)-1-[(2-Hydroxy-1-naphthyl)methylideneamino]imidazolidine-2,4-dione

Liang-Quan Sheng, Hua-Jie Xu, Na-Na Du and Xue-Yue Jiang

S1. Comment

The naphthalene group as a fluorophore has been studied extensively due to its characteristic photophysical properties and the competitive stability in the environment (Li *et al.*, 2010; Iijima *et al.*, 2010). As part of an ongoing study of Schiff bases incorporating the naphthalene group (Xu *et al.*, 2009), we report here on the crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. It can be seen to display a *trans* configuration about the C\bN bond. The bond lengths are normal (Allen *et al.*, 1987). There is an intramolecular O-H···N hydrogen bond (Table 1) and the molecule is relatively planar; dihedral angle involving the naphthalene mean plane and the imidazolidine-2,4-dione group mean plane being 8.4 (1)°. In the crystal structure of the title compound N—H···O intermolecular hydrongen bonds (Table 1) link two molecules to form dimmers situated about an inversion center. The molecules are further linked by weak C-H···O interactions to form a three-dimensional network (Fig. 2).

S2. Experimental

The solution of 1-Aminohydantoin hydrochloride (0.151 g, 1 mmol) in 5 ml of ethanol was added slowly to a solution containing 2-hydro-1- naphthaldehyde (0.172 g, 1 mmol) in 15 ml of absolute ethanol under heating and stirring. The mixture was then refluxed for 2 h. Afterwards the mixture was cooled to rt and the resulting solution to stand in air. After 15 days yellow block-shaped crystals were formed, on slow evaporation of the solvent.

S3. Refinement

The N3 H-atom was located in a difference Fourier map and freely refined: N-H = 0.89 (2) Å. All other H-atoms were placed in calculated positions and treated as riding: O—H = 0.82 Å, C—H = 0.93 or 0.97 Å, with U_{iso}(H) = 1.5 U_{eq}(parent O-atom) and = 1.2U_{eq}(parent C-atom).

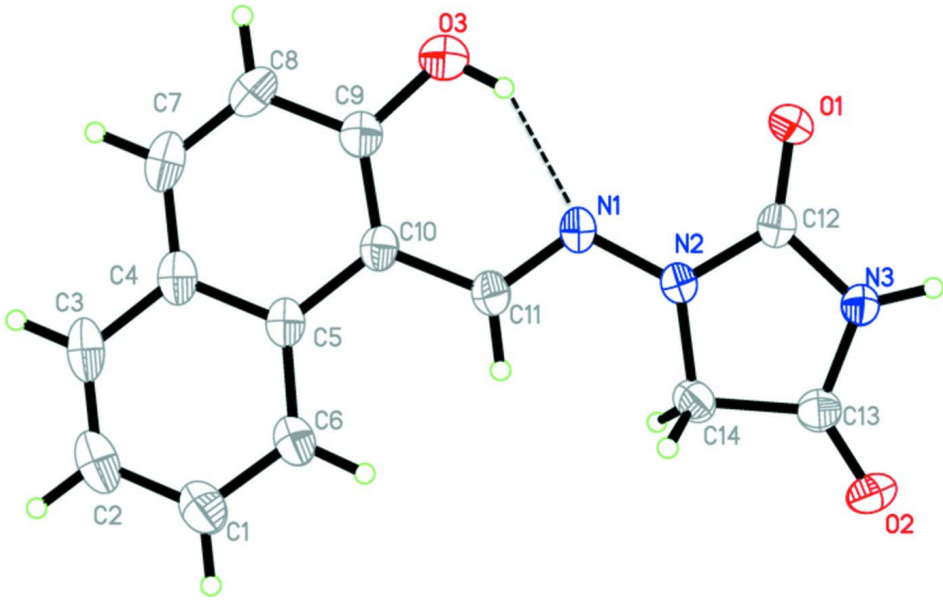

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids. The intramolecular O-H···N hydrogen bond is shown as a dashed line (see Table 1 for details).

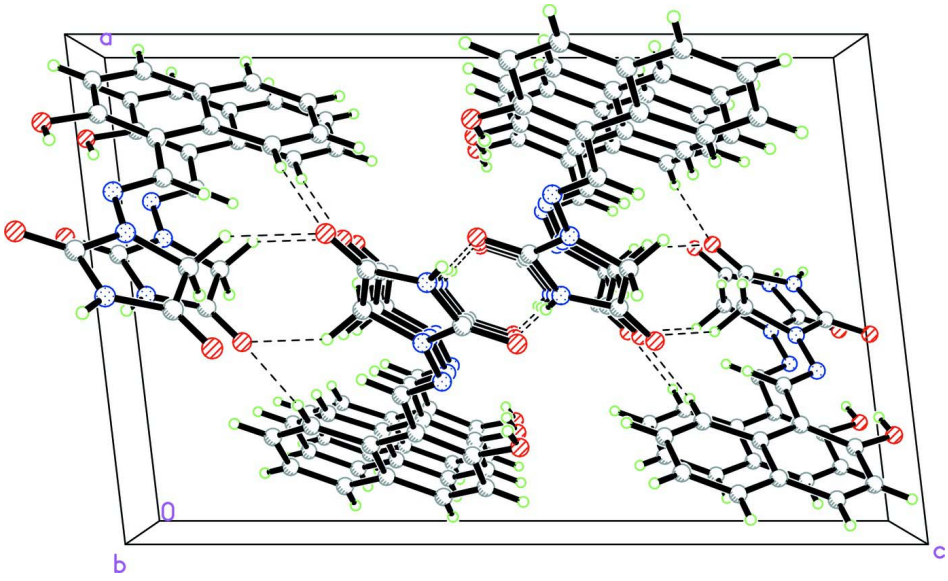

Figure 2

Crystal packing viewed along the b-axis of the title compound. The intra- and intermolecular hydrogen bonds are shown as dashed lines (see Table 1 for details).

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Crystal data

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Hall symbol: -P 2ybc
a = 11.5122 (7) Å
b = 6.0233 (3) Å

c = 17.9955 (10) Å
β = 96.773 (5)°
V = 1239.13 (12) Å^3
Z = 4
F(000) = 560
D_x = 1.443 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 1596 reflections
θ = 3.1–29.0°
μ = 0.11 mm^{-1}
T = 293 K
Block, yellow
0.40 × 0.30 × 0.30 mm

Data collection

Oxford Diffraction Gemini S Ultra diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 15.9149 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.959, T_{max} = 0.969

4288 measured reflections
2136 independent reflections
1053 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.0°, θ_{min} = 3.6°
h = −13→13
k = 0→6
l = 0→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.067
S = 0.72
2136 reflections
186 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
$w = 1/[\sigma^2(F_o^2) + (0.0266P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Special details

Experimental. Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm CrysAlisPro (Oxford Diffraction, 2009).

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

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 $F^2 > 2$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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.59888 (11)	0.25607 (18)	0.48396 (8)	0.0491 (5)
O2	0.40014 (13)	0.1526 (2)	0.68676 (8)	0.0710 (7)
O3	0.80499 (13)	0.8397 (2)	0.49453 (8)	0.0645 (6)
N1	0.67397 (13)	0.6177 (2)	0.57838 (9)	0.0420 (6)
N2	0.59925 (13)	0.4517 (2)	0.59460 (9)	0.0425 (6)
N3	0.48790 (15)	0.1552 (3)	0.57835 (10)	0.0454 (7)
C1	0.79653 (19)	1.2321 (3)	0.80751 (14)	0.0665 (10)

C2	0.8627 (2)	1.4184 (4)	0.79511 (16)	0.0705 (10)
C3	0.90328 (19)	1.4454 (3)	0.72772 (16)	0.0626 (9)
C4	0.87808 (17)	1.2884 (3)	0.66974 (14)	0.0504 (9)
C5	0.80840 (16)	1.1006 (3)	0.68128 (12)	0.0434 (8)
C6	0.77027 (17)	1.0762 (3)	0.75298 (13)	0.0549 (9)
C7	0.91986 (18)	1.3147 (3)	0.59955 (15)	0.0606 (10)
C8	0.89532 (17)	1.1653 (4)	0.54362 (13)	0.0589 (9)
C9	0.82579 (17)	0.9788 (3)	0.55419 (13)	0.0495 (9)
C10	0.78023 (16)	0.9449 (3)	0.62117 (12)	0.0413 (8)
C11	0.70303 (15)	0.7611 (3)	0.63076 (11)	0.0436 (7)
C12	0.56648 (16)	0.2867 (3)	0.54520 (12)	0.0398 (8)
C13	0.46509 (18)	0.2336 (3)	0.64613 (12)	0.0503 (9)
C14	0.53798 (18)	0.4406 (3)	0.66051 (11)	0.0496 (8)
H1	0.76960	1.21310	0.85380	0.0800*
H2	0.87910	1.52400	0.83260	0.0850*
H3	0.94840	1.56920	0.71970	0.0750*
H3N	0.4590 (16)	0.028 (3)	0.5590 (11)	0.065 (7)*
H4	0.76770	0.73180	0.50630	0.0970*
H6	0.72670	0.95210	0.76300	0.0660*
H7	0.96540	1.43790	0.59150	0.0730*
H8	0.92460	1.18630	0.49810	0.0710*
H11	0.67310	0.74520	0.67630	0.0520*
H14A	0.48920	0.57040	0.66440	0.0600*
H14B	0.59220	0.42690	0.70580	0.0600*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0538 (10)	0.0529 (8)	0.0415 (10)	−0.0044 (7)	0.0094 (8)	−0.0084 (7)
O2	0.0901 (13)	0.0776 (10)	0.0488 (11)	−0.0257 (9)	0.0233 (9)	0.0057 (9)
O3	0.0725 (12)	0.0686 (10)	0.0544 (11)	−0.0094 (8)	0.0156 (9)	−0.0054 (9)
N1	0.0401 (10)	0.0373 (9)	0.0473 (12)	−0.0016 (8)	0.0000 (9)	−0.0017 (9)
N2	0.0467 (11)	0.0387 (10)	0.0424 (12)	−0.0071 (9)	0.0067 (9)	−0.0046 (9)
N3	0.0522 (12)	0.0420 (11)	0.0421 (13)	−0.0091 (9)	0.0061 (10)	−0.0013 (10)
C1	0.0649 (16)	0.0670 (16)	0.0662 (18)	−0.0015 (14)	0.0014 (14)	−0.0187 (14)
C2	0.0648 (18)	0.0583 (16)	0.083 (2)	0.0033 (13)	−0.0137 (16)	−0.0216 (15)
C3	0.0477 (15)	0.0391 (13)	0.095 (2)	−0.0026 (11)	−0.0162 (15)	−0.0068 (15)
C4	0.0383 (14)	0.0375 (13)	0.0718 (18)	0.0023 (11)	−0.0083 (12)	0.0001 (13)
C5	0.0343 (12)	0.0361 (12)	0.0576 (16)	0.0059 (10)	−0.0042 (11)	−0.0009 (11)
C6	0.0523 (15)	0.0508 (14)	0.0602 (17)	−0.0031 (11)	0.0014 (13)	−0.0107 (13)
C7	0.0455 (15)	0.0441 (14)	0.090 (2)	−0.0063 (11)	−0.0017 (15)	0.0105 (14)
C8	0.0478 (14)	0.0590 (15)	0.0704 (18)	−0.0027 (12)	0.0097 (13)	0.0143 (14)
C9	0.0432 (14)	0.0457 (13)	0.0586 (17)	0.0027 (11)	0.0013 (12)	−0.0004 (12)
C10	0.0328 (12)	0.0372 (12)	0.0532 (15)	−0.0012 (10)	0.0017 (11)	0.0029 (11)
C11	0.0457 (13)	0.0405 (11)	0.0441 (14)	0.0024 (11)	0.0037 (11)	−0.0020 (11)
C12	0.0377 (13)	0.0386 (13)	0.0417 (14)	0.0016 (10)	−0.0010 (11)	0.0013 (11)
C13	0.0601 (16)	0.0494 (14)	0.0406 (15)	−0.0026 (12)	0.0029 (12)	0.0028 (12)
C14	0.0585 (15)	0.0488 (13)	0.0410 (14)	−0.0022 (11)	0.0036 (12)	−0.0052 (10)

Geometric parameters (Å, º)

O1—C12	1.219 (3)	C5—C10	1.440 (3)
O2—C13	1.209 (3)	C5—C6	1.419 (3)
O3—C9	1.361 (3)	C7—C8	1.355 (3)
O3—H4	0.8200	C8—C9	1.405 (3)
N1—N2	1.3726 (19)	C9—C10	1.385 (3)
N1—C11	1.293 (2)	C10—C11	1.443 (3)
N2—C12	1.357 (2)	C13—C14	1.508 (3)
N2—C14	1.451 (3)	C1—H1	0.9300
N3—C13	1.362 (3)	C2—H2	0.9300
N3—C12	1.389 (3)	C3—H3	0.9300
N3—H3N	0.890 (18)	C6—H6	0.9300
C1—C6	1.366 (3)	C7—H7	0.9300
C1—C2	1.389 (3)	C8—H8	0.9300
C2—C3	1.360 (4)	C11—H11	0.9300
C3—C4	1.413 (3)	C14—H14A	0.9700
C4—C7	1.413 (4)	C14—H14B	0.9700
C4—C5	1.416 (3)		
C9—O3—H4	109.00	N2—C12—N3	106.33 (17)
N2—N1—C11	116.51 (16)	O1—C12—N2	127.76 (17)
N1—N2—C14	125.77 (14)	O1—C12—N3	125.91 (18)
C12—N2—C14	112.17 (15)	O2—C13—N3	126.88 (18)
N1—N2—C12	121.80 (16)	O2—C13—C14	126.97 (19)
C12—N3—C13	113.02 (17)	N3—C13—C14	106.15 (17)
C13—N3—H3N	123.1 (13)	N2—C14—C13	102.24 (15)
C12—N3—H3N	123.7 (13)	C2—C1—H1	119.00
C2—C1—C6	121.3 (2)	C6—C1—H1	119.00
C1—C2—C3	119.5 (2)	C1—C2—H2	120.00
C2—C3—C4	121.1 (2)	C3—C2—H2	120.00
C3—C4—C5	119.8 (2)	C2—C3—H3	119.00
C3—C4—C7	121.57 (18)	C4—C3—H3	119.00
C5—C4—C7	118.64 (19)	C1—C6—H6	119.00
C4—C5—C10	119.44 (19)	C5—C6—H6	119.00
C4—C5—C6	117.23 (19)	C4—C7—H7	119.00
C6—C5—C10	123.33 (17)	C8—C7—H7	119.00
C1—C6—C5	121.07 (18)	C7—C8—H8	120.00
C4—C7—C8	121.78 (19)	C9—C8—H8	120.00
C7—C8—C9	120.2 (2)	N1—C11—H11	119.00
C8—C9—C10	121.05 (19)	C10—C11—H11	119.00
O3—C9—C10	123.12 (17)	N2—C14—H14A	111.00
O3—C9—C8	115.82 (19)	N2—C14—H14B	111.00
C5—C10—C9	118.88 (17)	C13—C14—H14A	111.00
C5—C10—C11	119.83 (18)	C13—C14—H14B	111.00
C9—C10—C11	121.27 (18)	H14A—C14—H14B	109.00
N1—C11—C10	122.37 (18)		

C11—N1—N2—C12	−177.23 (16)	C7—C4—C5—C10	−1.2 (3)
C11—N1—N2—C14	9.1 (2)	C3—C4—C7—C8	−179.6 (2)
N2—N1—C11—C10	−179.57 (16)	C5—C4—C7—C8	−0.2 (3)
N1—N2—C12—O1	2.8 (3)	C4—C5—C6—C1	2.3 (3)
N1—N2—C12—N3	−177.61 (15)	C10—C5—C6—C1	−178.07 (19)
C14—N2—C12—O1	177.26 (19)	C4—C5—C10—C9	2.3 (3)
C14—N2—C12—N3	−3.1 (2)	C4—C5—C10—C11	−175.93 (17)
N1—N2—C14—C13	176.87 (16)	C6—C5—C10—C9	−177.34 (18)
C12—N2—C14—C13	2.7 (2)	C6—C5—C10—C11	4.4 (3)
C13—N3—C12—O1	−178.02 (19)	C4—C7—C8—C9	0.6 (3)
C13—N3—C12—N2	2.4 (2)	C7—C8—C9—O3	179.31 (19)
C12—N3—C13—O2	179.8 (2)	C7—C8—C9—C10	0.6 (3)
C12—N3—C13—C14	−0.7 (2)	O3—C9—C10—C5	179.36 (17)
C6—C1—C2—C3	−0.7 (3)	O3—C9—C10—C11	−2.4 (3)
C2—C1—C6—C5	−0.9 (3)	C8—C9—C10—C5	−2.1 (3)
C1—C2—C3—C4	0.8 (3)	C8—C9—C10—C11	176.19 (18)
C2—C3—C4—C5	0.7 (3)	C5—C10—C11—N1	179.33 (17)
C2—C3—C4—C7	−179.9 (2)	C9—C10—C11—N1	1.1 (3)
C3—C4—C5—C6	−2.2 (3)	O2—C13—C14—N2	178.40 (19)
C3—C4—C5—C10	178.15 (18)	N3—C13—C14—N2	−1.1 (2)
C7—C4—C5—C6	178.47 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*N*···O1^{i}	0.890 (18)	1.962 (18)	2.851 (2)	177.9 (19)
O3—H4···N1	0.82	1.91	2.622 (2)	145
C6—H6···O2^{ii}	0.93	2.55	3.469 (2)	169
C14—H14*B*···O2^{ii}	0.97	2.36	3.038 (2)	127

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, *y*+1/2, −*z*+3/2.