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Keywords: crystal structure; hydrogen bonds; nitroxyl donor; oxime; non-conventional hydrogen bond.

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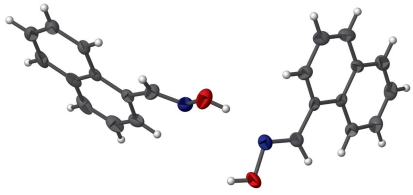
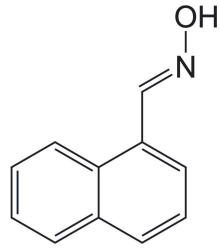
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{11}H_9NO$, crystallizes with two molecules, *A* and *B*, with similar conformations (r.m.s. overlay fit = 0.030 Å) in the asymmetric unit: the C—C═N···O torsion angles are −177.8 (3) and −179.1 (3)°. In the crystal, molecules are linked by alternating O—H···N (*A* → *B*) and O—H···O (*B* → *A*) hydrogen bonds to generate [100] chains. A weak C—H···O interaction is also observed.

3D view



Chemical scheme



Structure description

Compounds containing the oxime functional group have been the subject of interest for many years due to many their functions as synthetic congeners or precursors, as substrates for bioconjugation reaction (Kömel & Kool, 2017) and also as nitroxyl (HNO) donors (Sha *et al.*, 2006). Oximes are generally reactive; however, conjugation leads to an increase in stability of this functional group (Kömel, 2017), which is observed in the title compound that was studied as part of an undergraduate project devoted to single-crystal X-ray diffraction.

The title compound crystallizes in the orthorhombic crystal system, space group $P2_12_12_1$. There are two molecules, *A* (containing N1) and *B* (containing N2) in the asymmetric unit (Fig. 1). The bond distances for the oxime functional group are 1.281 (4) and 1.399 (4) Å for C1═N1 and N1—O1, respectively (molecule *A*) and 1.278 (5) and 1.401 (4) Å for C12═N2 and N2—O2, respectively (molecule *B*). The angle for C=N—O is 111.0 (3) (molecule *A*) and 111.3 (3)° (molecule *B*). These values are comparable to those in the same molecule co-crystallized with tetrabutylammonium cations and fluoride anions (Rosen *et al.*, 2013).

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.84 (2)	1.96 (2)	2.752 (4)	158 (3)
O2—H2···O1^{i}	0.84 (1)	2.00 (2)	2.808 (4)	163 (2)
C1—H1A···O2^{ii}	0.95 (1)	2.51 (1)	3.305 (5)	142 (1)

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

In the extended structure, O—H···N (A –> B) and O—H···O (B –> A) hydrogen bonds link the molecules into [100] chains (Table 1, Fig. 2). A weak C—H···O interaction is also observed.

Synthesis and crystallization

The title oxime was synthesized using the reported procedure of Rosen *et al.* (2013). Colourless needles were recrystallized from dichloromethane solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The absolute structure/chirality was indeterminate in the present refinement.

Funding information

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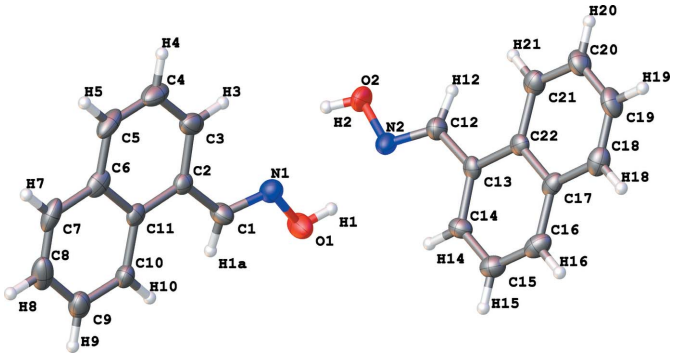

Figure 1
A view of the molecular structure, showing 50% probability displacement ellipsoids.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_9NO$
M_r	171.20
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
a, b, c (Å)	6.0506 (8), 13.7423 (18), 20.886 (3)
V (Å^3)	1736.7 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.50 × 0.10 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.678, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8745, 3390, 2106
R_{int}	0.077
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.069, 0.139, 1.04
No. of reflections	3390
No. of parameters	237
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.40, −0.46

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015), *olex2.refine* (Bourhis *et al.*, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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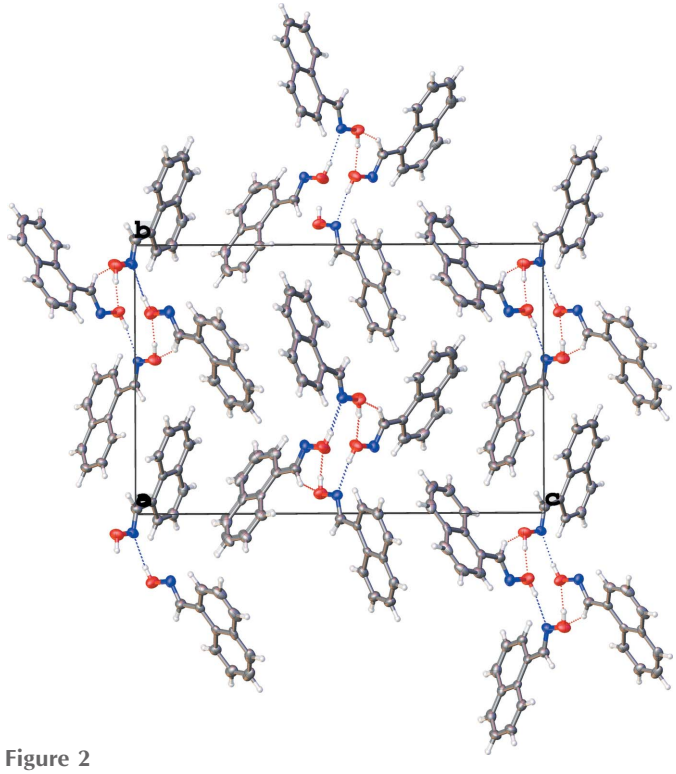

Figure 2
A view down [100] of the crystal packing. The hydrogen bonds are shown as dashed lines.

full crystallographic data

IUCrData (2017). **2**, x171720 [https://doi.org/10.1107/S2414314617017205]

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Naphthalene-1-carbaldehyde oxime

Crystal data

$C_{11}H_9NO$
M_r = 171.20
Orthorhombic, $P2_12_12_1$
a = 6.0506 (8) Å
b = 13.7423 (18) Å
c = 20.886 (3) Å
V = 1736.7 (4) Å^3
Z = 8
$F(000)$ = 720.3282
D_x = 1.309 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1679 reflections
θ = 3.1–27.3°
μ = 0.09 mm^{-1}
T = 150 K
Needle, clear colourless
0.50 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.678, T_{max} = 0.746
8745 measured reflections
3390 independent reflections
2106 reflections with $I > 2\sigma(I)$
R_{int} = 0.077
θ_{max} = 26.0°, θ_{min} = 3.3°
h = −7→7
k = −18→16
l = −26→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.139
S = 1.04
3390 reflections
237 parameters
0 restraints
36 constraints
Primary atom site location: dual
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.5394P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}
Absolute structure: unk

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.8084 (5)	0.74706 (19)	0.04014 (14)	0.0416 (8)
H1	0.823 (5)	0.8017 (9)	0.0227 (16)	0.0624 (11)*
N1	0.6345 (5)	0.7510 (2)	0.08423 (14)	0.0314 (8)

C1	0.5986 (7)	0.6671 (3)	0.10891 (17)	0.0315 (10)
H1a	0.6895 (7)	0.6136 (3)	0.09740 (17)	0.0378 (12)*
C2	0.4174 (6)	0.6533 (3)	0.15500 (17)	0.0256 (9)
C3	0.2503 (7)	0.7215 (3)	0.1597 (2)	0.0355 (10)
H3	0.2534 (7)	0.7774 (3)	0.1330 (2)	0.0426 (13)*
C4	0.0769 (7)	0.7093 (3)	0.2030 (2)	0.0421 (11)
H4	−0.0347 (7)	0.7577 (3)	0.2061 (2)	0.0505 (14)*
C5	0.0664 (7)	0.6287 (3)	0.2408 (2)	0.0415 (12)
H5	−0.0535 (7)	0.6211 (3)	0.2698 (2)	0.0498 (14)*
C6	0.2303 (7)	0.5570 (3)	0.23757 (16)	0.0313 (10)
C7	0.2237 (7)	0.4731 (3)	0.27754 (18)	0.0403 (11)
H7	0.1044 (7)	0.4645 (3)	0.30657 (18)	0.0484 (14)*
C8	0.3859 (8)	0.4055 (3)	0.27451 (19)	0.0452 (12)
H8	0.3778 (8)	0.3495 (3)	0.30107 (19)	0.0543 (15)*
C9	0.5660 (7)	0.4168 (3)	0.23276 (18)	0.0380 (11)
H9	0.6797 (7)	0.3691 (3)	0.23166 (18)	0.0456 (13)*
C10	0.5776 (7)	0.4967 (3)	0.19358 (18)	0.0301 (9)
H10	0.6994 (7)	0.5036 (3)	0.16521 (18)	0.0361 (11)*
C11	0.4108 (6)	0.5691 (3)	0.19476 (17)	0.0243 (9)
O2	0.5555 (5)	0.92557 (18)	−0.04725 (14)	0.0380 (7)
H2	0.507 (4)	0.8683 (8)	−0.0472 (17)	0.0570 (11)*
N2	0.7406 (5)	0.9316 (2)	−0.00713 (14)	0.0285 (8)
C12	0.7995 (6)	1.0199 (3)	0.00150 (17)	0.0297 (9)
H12	0.7167 (6)	1.0704 (3)	−0.01825 (17)	0.0356 (11)*
C13	0.9902 (6)	1.0455 (2)	0.04078 (16)	0.0244 (9)
C14	1.1498 (6)	0.9772 (3)	0.05384 (17)	0.0286 (9)
H14	1.1352 (6)	0.9136 (3)	0.03645 (17)	0.0343 (11)*
C15	1.3321 (7)	0.9985 (3)	0.09178 (17)	0.0335 (10)
H15	1.4389 (7)	0.9496 (3)	0.10032 (17)	0.0402 (12)*
C16	1.3585 (7)	1.0891 (3)	0.11676 (18)	0.0359 (10)
H16	1.4837 (7)	1.1031 (3)	0.14262 (18)	0.0431 (12)*
C17	1.2003 (6)	1.1630 (3)	0.10446 (16)	0.0270 (9)
C18	1.2236 (7)	1.2576 (3)	0.13064 (17)	0.0356 (11)
H18	1.3501 (7)	1.2724 (3)	0.15579 (17)	0.0428 (13)*
C19	1.0696 (8)	1.3274 (3)	0.12058 (19)	0.0383 (11)
H19	1.0872 (8)	1.3900 (3)	0.13919 (19)	0.0460 (13)*
C20	0.8845 (8)	1.3073 (3)	0.08279 (18)	0.0356 (11)
H20	0.7776 (8)	1.3568 (3)	0.07551 (18)	0.0428 (13)*
C21	0.8553 (7)	1.2169 (3)	0.05604 (18)	0.0322 (10)
H21	0.7290 (7)	1.2043 (3)	0.03031 (18)	0.0386 (12)*
C22	1.0139 (6)	1.1419 (3)	0.06679 (16)	0.0244 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0419 (17)	0.0351 (17)	0.0478 (17)	0.0067 (16)	0.0178 (16)	0.0087 (14)
N1	0.029 (2)	0.036 (2)	0.0295 (17)	0.0005 (18)	0.0009 (17)	0.0025 (16)
C1	0.035 (2)	0.026 (2)	0.034 (2)	0.006 (2)	0.003 (2)	0.0017 (18)

C2	0.023 (2)	0.025 (2)	0.029 (2)	−0.004 (2)	−0.0020 (19)	−0.0052 (17)
C3	0.029 (2)	0.032 (2)	0.046 (2)	0.001 (2)	−0.010 (2)	−0.005 (2)
C4	0.025 (2)	0.043 (3)	0.059 (3)	0.004 (2)	0.001 (3)	−0.019 (2)
C5	0.024 (2)	0.051 (3)	0.049 (3)	−0.011 (2)	0.012 (2)	−0.023 (2)
C6	0.027 (2)	0.044 (3)	0.023 (2)	−0.009 (2)	−0.0017 (19)	−0.0135 (19)
C7	0.034 (3)	0.055 (3)	0.032 (2)	−0.024 (3)	0.002 (2)	−0.002 (2)
C8	0.050 (3)	0.046 (3)	0.040 (3)	−0.020 (3)	−0.018 (2)	0.014 (2)
C9	0.035 (3)	0.036 (2)	0.042 (2)	−0.009 (2)	−0.009 (2)	0.006 (2)
C10	0.024 (2)	0.029 (2)	0.037 (2)	−0.006 (2)	−0.002 (2)	0.0026 (18)
C11	0.022 (2)	0.026 (2)	0.0246 (19)	−0.0066 (19)	−0.0037 (19)	−0.0070 (17)
O2	0.0285 (15)	0.0326 (15)	0.0530 (17)	−0.0075 (15)	−0.0088 (16)	−0.0036 (15)
N2	0.0243 (18)	0.0275 (18)	0.0336 (17)	0.0001 (16)	0.0037 (17)	−0.0038 (15)
C12	0.029 (2)	0.027 (2)	0.034 (2)	−0.0015 (19)	−0.002 (2)	−0.0004 (18)
C13	0.029 (2)	0.0231 (19)	0.0207 (18)	−0.0050 (18)	0.0014 (18)	0.0042 (16)
C14	0.029 (2)	0.028 (2)	0.029 (2)	0.006 (2)	0.002 (2)	0.0020 (18)
C15	0.029 (2)	0.039 (3)	0.033 (2)	0.005 (2)	0.000 (2)	0.002 (2)
C16	0.026 (2)	0.054 (3)	0.028 (2)	−0.001 (2)	−0.002 (2)	0.005 (2)
C17	0.022 (2)	0.037 (2)	0.0222 (19)	−0.0055 (19)	0.0010 (19)	0.0054 (18)
C18	0.037 (3)	0.043 (3)	0.027 (2)	−0.010 (2)	−0.001 (2)	0.000 (2)
C19	0.053 (3)	0.024 (2)	0.038 (2)	−0.005 (2)	0.005 (2)	−0.0056 (19)
C20	0.041 (3)	0.026 (2)	0.039 (2)	0.000 (2)	0.004 (2)	−0.004 (2)
C21	0.033 (3)	0.034 (2)	0.029 (2)	−0.005 (2)	−0.002 (2)	0.0068 (19)
C22	0.025 (2)	0.025 (2)	0.023 (2)	−0.0016 (18)	0.0026 (17)	0.0070 (16)

Geometric parameters (Å, º)

O1—H1	0.839 (18)	O2—H2	0.840 (13)
O1—N1	1.399 (4)	O2—N2	1.401 (4)
N1—C1	1.281 (4)	N2—C12	1.277 (4)
C1—H1a	0.9500 (6)	C12—H12	0.951 (6)
C1—C2	1.471 (5)	C12—C13	1.459 (5)
C2—C3	1.381 (5)	C13—C14	1.374 (5)
C2—C11	1.425 (5)	C13—C22	1.439 (5)
C3—H3	0.9500 (6)	C14—H14	0.949 (6)
C3—C4	1.395 (6)	C14—C15	1.389 (5)
C4—H4	0.951 (6)	C15—H15	0.950 (6)
C4—C5	1.362 (6)	C15—C16	1.359 (5)
C5—H5	0.950 (6)	C16—H16	0.950 (6)
C5—C6	1.401 (6)	C16—C17	1.418 (6)
C6—C7	1.424 (6)	C17—C18	1.418 (5)
C6—C11	1.421 (5)	C17—C22	1.405 (5)
C7—H7	0.950 (6)	C18—H18	0.950 (6)
C7—C8	1.352 (6)	C18—C19	1.353 (6)
C8—H8	0.951 (6)	C19—H19	0.951 (6)
C8—C9	1.404 (6)	C19—C20	1.398 (6)
C9—H9	0.950 (6)	C20—H20	0.950 (6)
C9—C10	1.371 (5)	C20—C21	1.374 (5)
C10—H10	0.950 (6)	C21—H21	0.950 (6)

C10—C11	1.418 (5)	C21—C22	1.426 (5)
N1—O1—H1	109 (2)	N2—O2—H2	110 (2)
C1—N1—O1	111.0 (3)	C12—N2—O2	111.3 (3)
H1a—C1—N1	119.8 (2)	H12—C12—N2	119.0 (2)
C2—C1—N1	120.4 (4)	C13—C12—N2	121.9 (4)
C2—C1—H1a	119.8 (2)	C13—C12—H12	119.0 (2)
C3—C2—C1	120.3 (3)	C14—C13—C12	120.2 (3)
C11—C2—C1	120.4 (3)	C22—C13—C12	120.9 (3)
C11—C2—C3	119.3 (4)	C22—C13—C14	118.9 (3)
H3—C3—C2	119.5 (2)	H14—C14—C13	119.1 (2)
C4—C3—C2	121.0 (4)	C15—C14—C13	121.8 (4)
C4—C3—H3	119.5 (3)	C15—C14—H14	119.1 (2)
H4—C4—C3	119.7 (3)	H15—C15—C14	119.8 (2)
C5—C4—C3	120.6 (4)	C16—C15—C14	120.4 (4)
C5—C4—H4	119.7 (3)	C16—C15—H15	119.8 (3)
H5—C5—C4	119.6 (3)	H16—C16—C15	119.8 (3)
C6—C5—C4	120.7 (4)	C17—C16—C15	120.4 (4)
C6—C5—H5	119.6 (2)	C17—C16—H16	119.8 (2)
C7—C6—C5	121.4 (4)	C18—C17—C16	121.3 (4)
C11—C6—C5	119.5 (4)	C22—C17—C16	119.7 (4)
C11—C6—C7	119.0 (4)	C22—C17—C18	119.0 (4)
H7—C7—C6	119.7 (3)	H18—C18—C17	119.3 (2)
C8—C7—C6	120.5 (4)	C19—C18—C17	121.4 (4)
C8—C7—H7	119.7 (3)	C19—C18—H18	119.3 (2)
H8—C8—C7	119.5 (3)	H19—C19—C18	120.0 (2)
C9—C8—C7	121.1 (4)	C20—C19—C18	120.0 (4)
C9—C8—H8	119.5 (3)	C20—C19—H19	120.0 (2)
H9—C9—C8	120.1 (3)	H20—C20—C19	119.6 (2)
C10—C9—C8	119.9 (4)	C21—C20—C19	120.7 (4)
C10—C9—H9	120.1 (3)	C21—C20—H20	119.6 (3)
H10—C10—C9	119.5 (3)	H21—C21—C20	119.9 (3)
C11—C10—C9	121.0 (4)	C22—C21—C20	120.2 (4)
C11—C10—H10	119.5 (2)	C22—C21—H21	119.9 (2)
C6—C11—C2	118.9 (3)	C17—C22—C13	118.8 (3)
C10—C11—C2	122.7 (3)	C21—C22—C13	122.6 (3)
C10—C11—C6	118.4 (3)	C21—C22—C17	118.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.84 (2)	1.96 (2)	2.752 (4)	158 (3)
O2—H2···O1^{i}	0.84 (1)	2.00 (2)	2.808 (4)	163 (2)
C1—H1A···O2^{ii}	0.95 (1)	2.51 (1)	3.305 (5)	142 (1)

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