Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Piperidinium 3-hydroxy-2-naphthoate

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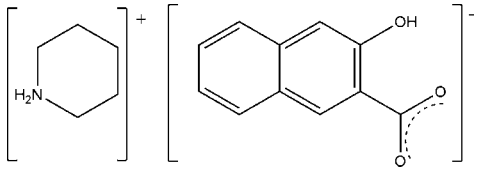
Received 30 July 2008; accepted 8 August 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.161; data-to-parameter ratio = 18.7.

The crystals of the title salt, $C_5H_{12}N^+\cdot C_{11}H_7O_3^-$, were obtained from a methanol/water solution of 3-hydroxy-2-naphthoic acid and piperidine at room temperature. In the crystal structure, the piperidinium cations display a chair conformation and link with hydroxynaphthoate anions *via* N—H···O and C—H···O hydrogen bonds. An intramolecular O—H···O interaction is also present.

Related literature

For background, see: Shen *et al.* (2008); Wang *et al.* (2005*a*,*b*, 2006).



Experimental

Crystal data

$C_5H_{12}N^+\cdot C_{11}H_7O_3^-$
M_r = 273.32
Monoclinic, $P2_1/n$
a = 8.6683 (3) Å
b = 19.4537 (5) Å
c = 9.5932 (3) Å
β = 111.959 (2)°
V = 1500.34 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
10640 measured reflections
3385 independent reflections
1512 reflections with $I > \sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.160
S = 0.99
3385 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 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
O1—H1B···O3	0.82	1.77	2.504 (2)	149
N1—H1C···O2^{i}	0.96	1.83	2.783 (2)	173
N1—H1D···O3	0.96	1.75	2.709 (2)	173
C12—H12A···O1^{ii}	0.97	2.40	3.336 (3)	161

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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*.

Y-TW thanks the Starting Fund of Shandong Institute of Light Industry for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2446).

References

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Wang, Y.-T., Tang, G.-M. & Qin, D.-W. (2005*a*). *Acta Cryst.* E**61**, o3623–o3624.
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supporting information

Acta Cryst. (2008). E**64**, o1753 [doi:10.1107/S1600536808025567]

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S1. Comment

In some biological system, intermolecular interactions play the important role (Shen *et al.*, 2008), these interactions have attracted our much attention in past years. A series of compounds with weak intermolecular interactions have been synthesized and their crystal structures have been characterized (Wang *et al.*, 2005a,b, 2006). As part of our investigation, we recently prepared the title compound and present here its crystal structure.

The molecular structure of the title compound is shown in Fig. 1. The asymmetric unit contains one 3-hydroxy-2-naphthoate anion and one piperidinium cation. The piperidinium cation displays a typical chair conformation. The carboxylate group is coplanar with the naphthalene ring. Intermolecular N—H···O and C—H···O hydrogen bonding presents in the crystal structure (Table 1).

S2. Experimental

3-Hydroxy-2-naphthoic acid (94 mg, 0.5 mmol) and piperidine (43 mg, 0.5 mmol) were dissolved in methanol (5 ml) and water (1 ml) at room temperature. The single crystals of the title compound were obtained from the solution after several days.

S3. Refinement

H atoms were placed in calculated positions with O—H = 0.82, N—H = 0.96, C—H = 0.93 (aromatic) or 0.97 Å (methylene), and refined in riding mode with U_{iso}(H) = 1.5U_{eq}(O,N) and 1.2U_{iso}(C).

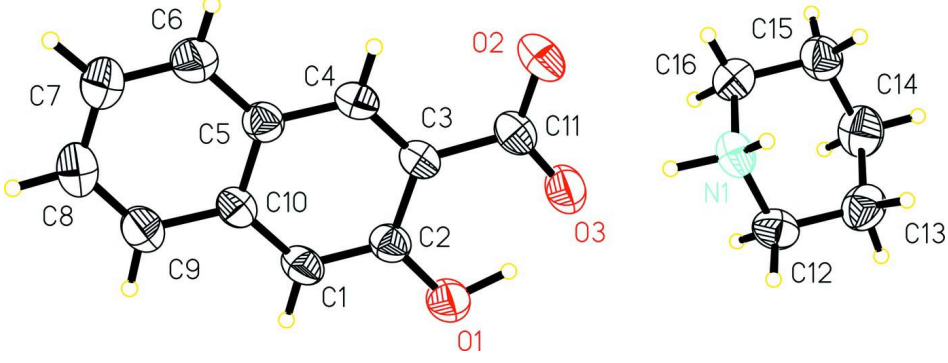

Figure 1

A drawing of (I), with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Piperidinium 3-hydroxy-2-naphthoate

Crystal data

$C_5H_{12}N^+·C_{11}H_7O_3^-$
M_r = 273.32
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 8.6683 (3) Å
b = 19.4537 (5) Å
c = 9.5932 (3) Å
β = 111.959 (2)°
V = 1500.34 (8) Å^3
Z = 4
$F(000)$ = 584
D_x = 1.210 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1627 reflections
θ = 2.5–20.5°
μ = 0.08 mm^{-1}
T = 298 K
Block, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
10640 measured reflections
3385 independent reflections
1512 reflections with $I > \sigma(I)$
R_{int} = 0.035
θ_{max} = 27.4°, θ_{min} = 2.1°
h = −9→11
k = −25→22
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.160
S = 0.99
3385 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0733P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	−0.1726 (2)	0.09197 (8)	0.39856 (18)	0.0718 (5)
H1C	−0.1979	0.0491	0.4346	0.108*
H1D	−0.0626	0.1054	0.4635	0.108*
O1	0.31760 (19)	0.22455 (7)	0.73435 (18)	0.0944 (5)
H1B	0.2331	0.2051	0.6786	0.142*

O2	0.24997 (18)	0.03674 (7)	0.51894 (15)	0.0832 (5)
O3	0.14101 (19)	0.13370 (8)	0.56381 (18)	0.0948 (5)
C1	0.6069 (3)	0.20988 (10)	0.8318 (2)	0.0692 (6)
H1A	0.6176	0.2530	0.8763	0.083*
C2	0.4523 (3)	0.18561 (9)	0.7481 (2)	0.0636 (5)
C3	0.4321 (2)	0.12071 (9)	0.67629 (19)	0.0561 (5)
C4	0.5718 (3)	0.08253 (9)	0.69633 (19)	0.0604 (5)
H4A	0.5597	0.0398	0.6498	0.072*
C5	0.7325 (3)	0.10544 (10)	0.7844 (2)	0.0629 (5)
C6	0.8758 (3)	0.06627 (12)	0.8062 (3)	0.0930 (7)
H6A	0.8654	0.0229	0.7626	0.112*
C7	1.0287 (3)	0.09073 (16)	0.8897 (3)	0.1178 (10)
H7A	1.1223	0.0642	0.9027	0.141*
C8	1.0468 (3)	0.15586 (15)	0.9569 (3)	0.1102 (9)
H8A	1.1524	0.1724	1.0137	0.132*
C9	0.9119 (3)	0.19463 (12)	0.9394 (2)	0.0838 (6)
H9A	0.9256	0.2375	0.9852	0.101*
C10	0.7497 (3)	0.17107 (10)	0.8523 (2)	0.0623 (5)
C11	0.2638 (3)	0.09412 (11)	0.5796 (2)	0.0669 (6)
C12	−0.2927 (3)	0.14545 (10)	0.4042 (2)	0.0772 (6)
H12A	−0.2619	0.1895	0.3749	0.093*
H12B	−0.2893	0.1495	0.5061	0.093*
C13	−0.4652 (3)	0.12680 (12)	0.3005 (3)	0.0900 (7)
H13A	−0.5412	0.1634	0.3004	0.108*
H13B	−0.5001	0.0853	0.3366	0.108*
C14	−0.4732 (3)	0.11527 (13)	0.1424 (3)	0.0995 (8)
H14A	−0.5837	0.0996	0.0798	0.119*
H14B	−0.4525	0.1583	0.1015	0.119*
C15	−0.3471 (3)	0.06288 (13)	0.1397 (2)	0.0857 (7)
H15A	−0.3759	0.0184	0.1690	0.103*
H15B	−0.3490	0.0589	0.0383	0.103*
C16	−0.1763 (3)	0.08263 (11)	0.2440 (3)	0.0852 (7)
H16A	−0.0979	0.0471	0.2439	0.102*
H16B	−0.1434	0.1251	0.2097	0.102*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0655 (12)	0.0642 (11)	0.0731 (11)	−0.0064 (8)	0.0116 (9)	0.0044 (8)
O1	0.0755 (11)	0.0761 (10)	0.1167 (13)	0.0101 (8)	0.0186 (9)	−0.0260 (8)
O2	0.0942 (12)	0.0604 (9)	0.0768 (10)	−0.0154 (7)	0.0110 (8)	−0.0074 (7)
O3	0.0677 (11)	0.0869 (11)	0.1111 (13)	−0.0032 (9)	0.0121 (9)	−0.0172 (9)
C1	0.0774 (16)	0.0539 (11)	0.0683 (13)	−0.0059 (11)	0.0182 (12)	−0.0120 (9)
C2	0.0689 (15)	0.0538 (12)	0.0641 (12)	0.0031 (11)	0.0203 (11)	−0.0032 (9)
C3	0.0682 (14)	0.0483 (10)	0.0481 (10)	−0.0035 (9)	0.0176 (9)	0.0014 (8)
C4	0.0753 (15)	0.0505 (11)	0.0529 (11)	−0.0009 (10)	0.0211 (10)	−0.0031 (8)
C5	0.0656 (14)	0.0660 (13)	0.0545 (11)	0.0015 (11)	0.0192 (10)	−0.0012 (9)
C6	0.0789 (19)	0.0897 (16)	0.0979 (17)	0.0125 (14)	0.0187 (14)	−0.0205 (13)

C7	0.071 (2)	0.130 (2)	0.131 (2)	0.0165 (16)	0.0138 (17)	−0.0327 (19)
C8	0.0669 (19)	0.126 (2)	0.119 (2)	−0.0029 (16)	0.0122 (15)	−0.0265 (18)
C9	0.0794 (17)	0.0836 (15)	0.0786 (15)	−0.0114 (13)	0.0181 (13)	−0.0138 (12)
C10	0.0655 (14)	0.0637 (13)	0.0536 (11)	−0.0056 (10)	0.0174 (10)	−0.0023 (9)
C11	0.0755 (16)	0.0566 (13)	0.0604 (12)	−0.0084 (12)	0.0160 (11)	0.0031 (10)
C12	0.1010 (19)	0.0594 (13)	0.0748 (14)	−0.0006 (12)	0.0371 (14)	0.0028 (10)
C13	0.0788 (18)	0.0879 (16)	0.1040 (19)	0.0125 (13)	0.0351 (15)	0.0085 (14)
C14	0.0805 (18)	0.116 (2)	0.0847 (17)	0.0087 (15)	0.0112 (13)	0.0173 (15)
C15	0.0853 (19)	0.1038 (18)	0.0645 (13)	−0.0124 (14)	0.0239 (13)	−0.0070 (12)
C16	0.0800 (18)	0.0910 (16)	0.0915 (16)	−0.0034 (13)	0.0401 (14)	−0.0088 (13)

Geometric parameters (Å, º)

N1—C12	1.487 (2)	C7—C8	1.403 (3)
N1—C16	1.482 (3)	C7—H7A	0.9300
N1—H1C	0.9601	C8—C9	1.348 (3)
N1—H1D	0.9600	C8—H8A	0.9300
O1—C2	1.357 (2)	C9—C10	1.417 (3)
O1—H1B	0.8200	C9—H9A	0.9300
O2—C11	1.244 (2)	C12—C13	1.498 (3)
O3—C11	1.276 (2)	C12—H12A	0.9700
C1—C2	1.363 (3)	C12—H12B	0.9700
C1—C10	1.400 (3)	C13—C14	1.509 (3)
C1—H1A	0.9300	C13—H13A	0.9700
C2—C3	1.417 (2)	C13—H13B	0.9700
C3—C4	1.372 (3)	C14—C15	1.502 (3)
C3—C11	1.498 (3)	C14—H14A	0.9700
C4—C5	1.404 (3)	C14—H14B	0.9700
C4—H4A	0.9300	C15—C16	1.494 (3)
C5—C6	1.404 (3)	C15—H15A	0.9700
C5—C10	1.416 (2)	C15—H15B	0.9700
C6—C7	1.353 (3)	C16—H16A	0.9700
C6—H6A	0.9300	C16—H16B	0.9700
C12—N1—C16	111.63 (16)	C1—C10—C9	122.6 (2)
C12—N1—H1C	109.7	C5—C10—C9	118.3 (2)
C16—N1—H1C	109.4	O2—C11—O3	123.8 (2)
C12—N1—H1D	108.9	O2—C11—C3	120.0 (2)
C16—N1—H1D	109.2	O3—C11—C3	116.16 (19)
H1C—N1—H1D	108.0	N1—C12—C13	110.18 (17)
C2—O1—H1B	109.5	N1—C12—H12A	109.6
C2—C1—C10	121.22 (18)	C13—C12—H12A	109.6
C2—C1—H1A	119.4	N1—C12—H12B	109.6
C10—C1—H1A	119.4	C13—C12—H12B	109.6
O1—C2—C1	118.97 (18)	H12A—C12—H12B	108.1
O1—C2—C3	120.30 (19)	C12—C13—C14	111.27 (19)
C1—C2—C3	120.74 (19)	C12—C13—H13A	109.4
C4—C3—C2	118.14 (18)	C14—C13—H13A	109.4

C4—C3—C11	120.27 (18)	C12—C13—H13B	109.4
C2—C3—C11	121.58 (19)	C14—C13—H13B	109.4
C3—C4—C5	122.53 (18)	H13A—C13—H13B	108.0
C3—C4—H4A	118.7	C15—C14—C13	110.99 (19)
C5—C4—H4A	118.7	C15—C14—H14A	109.4
C6—C5—C4	122.70 (19)	C13—C14—H14A	109.4
C6—C5—C10	119.1 (2)	C15—C14—H14B	109.4
C4—C5—C10	118.21 (18)	C13—C14—H14B	109.4
C7—C6—C5	120.9 (2)	H14A—C14—H14B	108.0
C7—C6—H6A	119.6	C16—C15—C14	111.0 (2)
C5—C6—H6A	119.6	C16—C15—H15A	109.4
C6—C7—C8	120.4 (2)	C14—C15—H15A	109.4
C6—C7—H7A	119.8	C16—C15—H15B	109.4
C8—C7—H7A	119.8	C14—C15—H15B	109.4
C9—C8—C7	120.3 (2)	H15A—C15—H15B	108.0
C9—C8—H8A	119.8	N1—C16—C15	110.30 (17)
C7—C8—H8A	119.8	N1—C16—H16A	109.6
C8—C9—C10	121.0 (2)	C15—C16—H16A	109.6
C8—C9—H9A	119.5	N1—C16—H16B	109.6
C10—C9—H9A	119.5	C15—C16—H16B	109.6
C1—C10—C5	119.13 (19)	H16A—C16—H16B	108.1

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···O3	0.82	1.77	2.504 (2)	149
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