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# Ammonium 1-hydroxy-2-naphthoate

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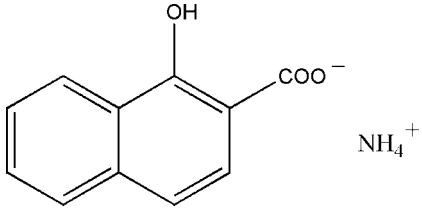
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.080; $wR$ factor = 0.227; data-to-parameter ratio = 12.9.

The title compound, $NH_4^+\cdot C_{11}H_7O_3^-$, was obtained by slow evaporation of a 30% ammonia solution of 1-hydroxy-2-naphthoic acid. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds, forming layers parallel to the *bc* plane.

## Related literature

For related literature, see: Kickelbick & Schubert (1999); Ohki *et al.* (1986); Song *et al.* (2008).




## Experimental

### Crystal data

$NH_4^+\cdot C_{11}H_7O_3^-$
$M_r$ = 205.21
Monoclinic, $C2/c$
$a$ = 30.883 (5) Å
$b$ = 3.880 (1) Å
$c$ = 15.777 (3) Å
$\beta$ = 95.567 (2)°
$V$ = 1881.6 (7) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 298 (2) K
0.23 × 0.23 × 0.20 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.976, $T_{max}$ = 0.979
6728 measured reflections
1915 independent reflections
1351 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.226
$S$ = 1.04
1915 reflections
149 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O2 | 0.82 | 1.73 | 2.463 (3) | 148 |
| N1—H1$A$···O1$^{i}$ | 0.89 (2) | 2.07 (3) | 2.920 (3) | 161 (3) |
| N1—H1$B$···O2$^{ii}$ | 0.89 (3) | 1.88 (3) | 2.756 (3) | 167 (3) |
| N1—H1$C$···O3$^{iii}$ | 0.89 (2) | 2.04 (2) | 2.789 (3) | 141 (3) |
| N1—H1$D$···O3$^{iv}$ | 0.88 (3) | 2.08 (2) | 2.821 (3) | 140 (3) |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2202).

## References

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# supplementary materials

*Acta Cryst.* (2008). E**64**, o813 [ **doi:10.1107/S1600536808009082** ]

# Ammonium 1-hydroxy-2-naphthoate

**Y. Bi and C.-L. Han**

## Comment

1-Hydroxynaphthalene-2-carboxylic acid is a widely used ligand for the synthesis of metal complexes (Kickelbick & Schubert, 1999; Ohki *et al.*, 1986; Song *et al.*, 2008). We report herein the crystal structure of the title compound, which was obtained by slow evaporation of a 30% ammonium solution of 1-hydroxynaphthalene-2-carboxylic acid in air.

The compound consists of discrete 1-hydroxynaphthalene-2-carboxylate anions and ammonium cations (Fig. 1). The anion is substantially planar with a mean deviation of 0.015 (3) Å. The crystal structure is stabilized by intermolecular N–H···O hydrogen bonds (Table 1), forming layers parallel to the *bc* plane (Fig. 2).

## Experimental

Single crystals of the title compound were obtained by slow evaporation of a 30% ammonia solution of 1-hydroxynaphthalene-2-carboxylic acid in air.

## Refinement

Ammonium H atoms were located from a difference Fourier map and refined isotropically, with N–H distances restrained to 0.90 (1) Å, H···H distances restrained to 1.43 (2) Å, and with $U_{iso}$(H) values fixed at 0.08 Å$^2$. All other H atoms were placed in idealized positions and constrained to ride on their parent atoms with C–H distances of 0.93 Å, O–H distance of 0.82 Å, and with $U_{iso}$(H) set at 1.2$U_{eq}$(C) or 1.5$U_{eq}$(O).

## Figures

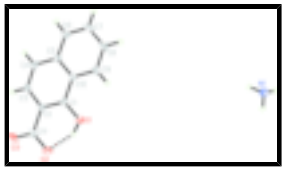

Fig. 1. The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular hydrogen bond is shown as a dashed line.

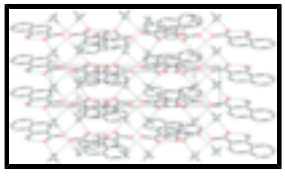

Fig. 2. A perspective view of crystal packing of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

### Ammonium 1-hydroxy-2-naphthoate

*Crystal data*

| | |
|---|---|
| $N_1H_4^+ \cdot C_{11}H_7O_3^-$ | $F_{000} = 864$ |
| $M_r = 205.21$ | $D_x = 1.449$ Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 1379 reflections |
| *a* = 30.883 (5) Å | θ = 2.5–24.1° |
| *b* = 3.880 (1) Å | μ = 0.11 mm$^{-1}$ |
| *c* = 15.777 (3) Å | *T* = 298 (2) K |
| β = 95.567 (2)° | Block, colourless |
| *V* = 1881.6 (7) Å$^3$ | 0.23 × 0.23 × 0.20 mm |
| *Z* = 8 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 1915 independent reflections |
| Radiation source: fine-focus sealed tube | 1351 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.040$ |
| *T* = 298(2) K | $\theta_{max} = 27.0°$ |
| ω scans | $\theta_{min} = 2.6°$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | *h* = −38→38 |
| $T_{min} = 0.976$, $T_{max} = 0.979$ | *k* = −4→4 |
| 6728 measured reflections | *l* = −20→19 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.080$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.226$ | $w = 1/[\sigma^2(F_o^2) + (0.1461P)^2 + 0.0944P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 1.04 | $(\Delta/\sigma)_{max} < 0.001$ |
| 1915 reflections | $\Delta\rho_{max} = 0.55$ e Å$^{-3}$ |
| 149 parameters | $\Delta\rho_{min} = -0.24$ e Å$^{-3}$ |
| 10 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.42976 (6) | 1.0366 (6) | 0.70025 (11) | 0.0383 (6) |
| H1 | 0.4496 | 1.0981 | 0.7354 | 0.057* |
| O2 | 0.46982 (6) | 1.1294 (6) | 0.84111 (13) | 0.0472 (6) |
| O3 | 0.44313 (7) | 0.9570 (6) | 0.95912 (12) | 0.0486 (7) |
| N1 | 0.46529 (8) | 0.4511 (7) | 0.08424 (16) | 0.0414 (7) |
| C1 | 0.39678 (8) | 0.9092 (6) | 0.74083 (16) | 0.0259 (6) |
| C2 | 0.39995 (8) | 0.8798 (7) | 0.82806 (16) | 0.0281 (6) |
| C3 | 0.36469 (8) | 0.7397 (7) | 0.86694 (16) | 0.0322 (6) |
| H3 | 0.3666 | 0.7214 | 0.9260 | 0.039* |
| C4 | 0.32803 (9) | 0.6309 (8) | 0.82012 (17) | 0.0354 (7) |
| H4 | 0.3052 | 0.5392 | 0.8474 | 0.042* |
| C5 | 0.32420 (8) | 0.6559 (7) | 0.73053 (17) | 0.0291 (6) |
| C6 | 0.28703 (9) | 0.5425 (7) | 0.67931 (19) | 0.0380 (7) |
| H6 | 0.2640 | 0.4471 | 0.7050 | 0.046* |
| C7 | 0.28423 (9) | 0.5700 (8) | 0.5933 (2) | 0.0441 (8) |
| H7 | 0.2594 | 0.4931 | 0.5606 | 0.053* |
| C8 | 0.31858 (10) | 0.7139 (8) | 0.55356 (18) | 0.0424 (8) |
| H8 | 0.3165 | 0.7321 | 0.4945 | 0.051* |
| C9 | 0.35487 (9) | 0.8268 (8) | 0.60050 (17) | 0.0358 (7) |
| H9 | 0.3773 | 0.9242 | 0.5733 | 0.043* |
| C10 | 0.35900 (8) | 0.7985 (7) | 0.68970 (16) | 0.0268 (6) |
| C11 | 0.43967 (9) | 0.9947 (7) | 0.88135 (17) | 0.0321 (7) |
| H1A | 0.4533 (9) | 0.347 (7) | 0.1262 (14) | 0.080* |
| H1B | 0.4891 (7) | 0.565 (8) | 0.1041 (18) | 0.080* |
| H1C | 0.4720 (10) | 0.291 (6) | 0.0471 (16) | 0.080* |
| H1D | 0.4467 (8) | 0.597 (7) | 0.0576 (18) | 0.080* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0294 (10) | 0.0542 (14) | 0.0317 (10) | −0.0088 (9) | 0.0045 (8) | 0.0017 (9) |
| O2 | 0.0307 (10) | 0.0587 (15) | 0.0509 (13) | −0.0139 (9) | −0.0027 (9) | −0.0017 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O3 | 0.0537 (13) | 0.0560 (15) | 0.0326 (11) | −0.0071 (10) | −0.0135 (10) | −0.0059 (10) |
| N1 | 0.0445 (14) | 0.0356 (14) | 0.0439 (14) | −0.0050 (11) | 0.0037 (12) | −0.0057 (11) |
| C1 | 0.0240 (12) | 0.0254 (13) | 0.0293 (13) | 0.0014 (9) | 0.0070 (10) | −0.0002 (10) |
| C2 | 0.0273 (13) | 0.0253 (14) | 0.0310 (13) | 0.0001 (10) | 0.0003 (10) | −0.0035 (10) |
| C3 | 0.0371 (14) | 0.0330 (15) | 0.0269 (13) | −0.0017 (12) | 0.0057 (11) | 0.0026 (11) |
| C4 | 0.0329 (14) | 0.0391 (17) | 0.0352 (14) | −0.0060 (11) | 0.0085 (12) | 0.0052 (12) |
| C5 | 0.0246 (12) | 0.0264 (14) | 0.0359 (14) | 0.0022 (10) | 0.0010 (10) | 0.0016 (11) |
| C6 | 0.0306 (14) | 0.0337 (16) | 0.0488 (16) | −0.0029 (11) | −0.0010 (12) | −0.0043 (13) |
| C7 | 0.0338 (15) | 0.0469 (19) | 0.0480 (17) | 0.0026 (12) | −0.0146 (13) | −0.0136 (14) |
| C8 | 0.0440 (16) | 0.0515 (19) | 0.0289 (14) | 0.0107 (14) | −0.0100 (12) | −0.0052 (13) |
| C9 | 0.0343 (14) | 0.0436 (17) | 0.0300 (14) | 0.0060 (12) | 0.0049 (11) | −0.0019 (12) |
| C10 | 0.0263 (12) | 0.0239 (13) | 0.0297 (13) | 0.0024 (10) | 0.0000 (10) | −0.0007 (10) |
| C11 | 0.0346 (14) | 0.0271 (14) | 0.0331 (14) | −0.0008 (11) | −0.0044 (11) | −0.0041 (11) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.349 (3) | C3—H3 | 0.9300 |
| O1—H1 | 0.8200 | C4—C5 | 1.410 (4) |
| O2—C11 | 1.287 (3) | C4—H4 | 0.9300 |
| O3—C11 | 1.230 (3) | C5—C6 | 1.409 (4) |
| N1—H1A | 0.89 (2) | C5—C10 | 1.418 (4) |
| N1—H1B | 0.89 (3) | C6—C7 | 1.356 (4) |
| N1—H1C | 0.89 (2) | C6—H6 | 0.9300 |
| N1—H1D | 0.88 (3) | C7—C8 | 1.400 (4) |
| C1—C2 | 1.375 (4) | C7—H7 | 0.9300 |
| C1—C10 | 1.419 (3) | C8—C9 | 1.355 (4) |
| C2—C3 | 1.410 (3) | C8—H8 | 0.9300 |
| C2—C11 | 1.487 (3) | C9—C10 | 1.405 (4) |
| C3—C4 | 1.358 (4) | C9—H9 | 0.9300 |
| C1—O1—H1 | 109.5 | C6—C5—C10 | 118.2 (3) |
| H1A—N1—H1B | 110.8 (19) | C4—C5—C10 | 119.3 (2) |
| H1A—N1—H1C | 108 (2) | C7—C6—C5 | 121.3 (3) |
| H1B—N1—H1C | 110.0 (19) | C7—C6—H6 | 119.4 |
| H1A—N1—H1D | 110 (2) | C5—C6—H6 | 119.4 |
| H1B—N1—H1D | 109 (2) | C6—C7—C8 | 120.1 (3) |
| H1C—N1—H1D | 108.3 (19) | C6—C7—H7 | 119.9 |
| O1—C1—C2 | 121.5 (2) | C8—C7—H7 | 119.9 |
| O1—C1—C10 | 117.3 (2) | C9—C8—C7 | 120.5 (3) |
| C2—C1—C10 | 121.2 (2) | C9—C8—H8 | 119.8 |
| C1—C2—C3 | 119.0 (2) | C7—C8—H8 | 119.8 |
| C1—C2—C11 | 121.1 (2) | C8—C9—C10 | 120.8 (3) |
| C3—C2—C11 | 120.0 (2) | C8—C9—H9 | 119.6 |
| C4—C3—C2 | 121.4 (2) | C10—C9—H9 | 119.6 |
| C4—C3—H3 | 119.3 | C9—C10—C5 | 119.1 (2) |
| C2—C3—H3 | 119.3 | C9—C10—C1 | 122.4 (2) |
| C3—C4—C5 | 120.5 (2) | C5—C10—C1 | 118.5 (2) |
| C3—C4—H4 | 119.7 | O3—C11—O2 | 122.9 (2) |
| C5—C4—H4 | 119.7 | O3—C11—C2 | 121.0 (3) |
| C6—C5—C4 | 122.5 (3) | O2—C11—C2 | 116.1 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O2 | 0.82 | 1.73 | 2.463 (3) | 148 |
| N1—H1A···O1$^{i}$ | 0.89 (2) | 2.07 (3) | 2.920 (3) | 161 (3) |
| N1—H1B···O2$^{ii}$ | 0.89 (3) | 1.88 (3) | 2.756 (3) | 167 (3) |
| N1—H1C···O3$^{iii}$ | 0.89 (2) | 2.04 (2) | 2.789 (3) | 141 (3) |
| N1—H1D···O3$^{iv}$ | 0.88 (3) | 2.08 (2) | 2.821 (3) | 140 (3) |

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

**Fig. 1**

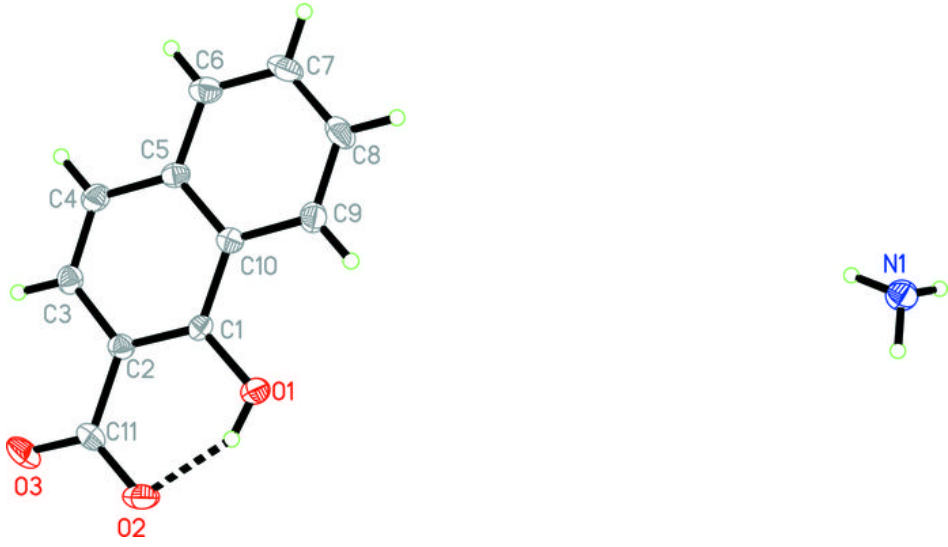

**Fig. 2**