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# 2-Methoxynaphthalene-1-carbaldehyde

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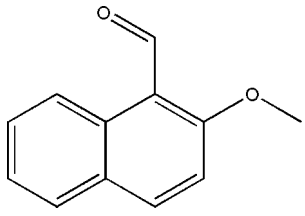
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.043; $wR$ factor = 0.124; data-to-parameter ratio = 16.0.

In the title compound, $C_{12}H_{10}O_2$, the aldehyde and methoxy groups are slightly twisted around the single bonds that join them to the naphthalene ring system. In the crystal structure, molecules are linked through intermolecular C—H···O hydrogen bonds, forming chains running along the $c$ axis.

## Related literature

For crystal structures of Schiff bases, see: Yehye *et al.* (2008); Tabatabaee *et al.* (2007); Zhang & Li (2007). For bond-length data, see: Allen *et al.* (1987).



## Experimental

### *Crystal data*

$C_{12}H_{10}O_2$
$M_r$ = 186.20
Monoclinic, $P2_1/c$
$a$ = 8.689 (3) Å
$b$ = 14.155 (4) Å
$c$ = 7.667 (2) Å
$\beta$ = 94.805 (4)°
$V$ = 939.7 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 298 K
0.20 × 0.20 × 0.18 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.982, $T_{max}$ = 0.984
5187 measured reflections
2046 independent reflections
1477 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.124
$S$ = 1.03
2046 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C12—H12$C$···O1$^{i}$ | 0.96 | 2.46 | 3.362 (4) | 156 (6) |

Symmetry code: (i) $x, y, z+1$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: CI2783).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, o1088 [ **doi:10.1107/S1600536809014287** ]

# 2-Methoxynaphthalene-1-carbaldehyde

**C. Tang**

## Comment

A large number of aldehydes were chosen as starting materials for the synthesis of Schiff base derivatives (Yehye *et al.*, 2008; Tabatabaee *et al.*, 2007; Zhang & Li, 2007). We report here the crystal structure of the title compound.

In the title molecule (Fig. 1), the bond lengths are within normal ranges (Allen *et al.*, 1987). The carbonyl oxygen atom O1 deviates from the plane of the naphthalene ring system by 0.027 (2) Å. The aldehyde and methoxy groups are slightly twisted away from the naphthalene ring system [C10—C1—C11—O1 10.6 (3)° and C12—O2—C2—C3 = 8.4 (2)°].

In the crystal structure, molecules are linked through intermolecular C–H···O hydrogen bonds (Table 1), forming chains running along the *c* axis (Fig. 2).

## Experimental

The title compound was obtained commercially (Lancaster). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution of the compound.

## Refinement

H atoms were positioned geometrically and refined as riding, with C-H = 0.93–0.96 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.5$U_{eq}$(C12).

## Figures

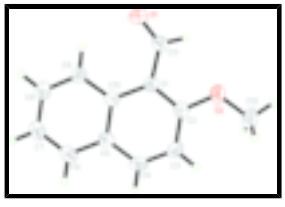

Fig. 1. The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

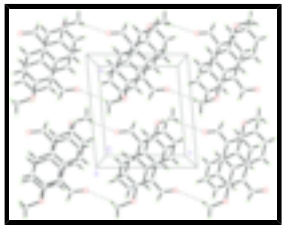

Fig. 2. The molecular packing of the title compound, viewed along the *b* axis. Intermolecular C–H···O hydrogen bonds are shown as dashed lines.

## 2-Methoxynaphthalene-1-carbaldehyde

*Crystal data*

| | |
|---|---|
| $C_{12}H_{10}O_2$ | $F_{000}$ = 392 |
| $M_r$ = 186.20 | $D_x$ = 1.316 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 1550 reflections |
| $a$ = 8.689 (3) Å | θ = 2.3–25.3º |
| $b$ = 14.155 (4) Å | μ = 0.09 mm$^{-1}$ |
| $c$ = 7.667 (2) Å | $T$ = 298 K |
| β = 94.805 (4)º | Block, colourless |
| $V$ = 939.7 (5) Å$^3$ | 0.20 × 0.20 × 0.18 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2046 independent reflections |
| Radiation source: fine-focus sealed tube | 1477 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.018 |
| $T$ = 298 K | $\theta_{max}$ = 27.0º |
| ω scans | $\theta_{min}$ = 2.4º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −8→11 |
| $T_{min}$ = 0.982, $T_{max}$ = 0.984 | $k$ = −17→18 |
| 5187 measured reflections | $l$ = −8→9 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.043 | H-atom parameters constrained |
| $wR(F^2)$ = 0.124 | $w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.1007P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.03 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 2046 reflections | $\Delta\rho_{max}$ = 0.12 e Å$^{-3}$ |
| 128 parameters | $\Delta\rho_{min}$ = −0.17 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*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 | 0.28487 (13) | 0.04582 (12) | −0.30026 (16) | 0.0951 (5) |
| O2 | 0.37442 (12) | 0.12897 (9) | 0.17417 (14) | 0.0716 (4) |
| C1 | 0.17514 (14) | 0.10308 (9) | −0.04428 (17) | 0.0445 (3) |
| C2 | 0.22015 (16) | 0.13172 (9) | 0.12545 (18) | 0.0493 (3) |
| C3 | 0.11126 (18) | 0.16328 (10) | 0.23780 (19) | 0.0570 (4) |
| H3 | 0.1427 | 0.1806 | 0.3523 | 0.068* |
| C4 | −0.03974 (18) | 0.16829 (10) | 0.17843 (19) | 0.0561 (4) |
| H4 | −0.1109 | 0.1892 | 0.2539 | 0.067* |
| C5 | −0.09270 (15) | 0.14282 (9) | 0.00617 (18) | 0.0467 (3) |
| C6 | −0.25038 (17) | 0.15016 (10) | −0.0548 (2) | 0.0596 (4) |
| H6 | −0.3211 | 0.1723 | 0.0200 | 0.072* |
| C7 | −0.29984 (17) | 0.12527 (11) | −0.2210 (2) | 0.0644 (4) |
| H7 | −0.4038 | 0.1305 | −0.2597 | 0.077* |
| C8 | −0.19430 (18) | 0.09191 (11) | −0.3336 (2) | 0.0617 (4) |
| H8 | −0.2289 | 0.0748 | −0.4473 | 0.074* |
| C9 | −0.04112 (16) | 0.08386 (10) | −0.28015 (18) | 0.0527 (4) |
| H9 | 0.0269 | 0.0613 | −0.3578 | 0.063* |
| C10 | 0.01568 (14) | 0.10936 (8) | −0.10843 (17) | 0.0426 (3) |
| C11 | 0.29521 (17) | 0.06484 (12) | −0.1473 (2) | 0.0618 (4) |
| H11 | 0.3909 | 0.0540 | −0.0870 | 0.074* |
| C12 | 0.4284 (2) | 0.14661 (15) | 0.3509 (2) | 0.0850 (6) |
| H12A | 0.4022 | 0.2100 | 0.3816 | 0.128* |
| H12B | 0.5385 | 0.1389 | 0.3649 | 0.128* |
| H12C | 0.3809 | 0.1029 | 0.4257 | 0.128* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0651 (8) | 0.1637 (14) | 0.0584 (8) | 0.0113 (7) | 0.0161 (6) | −0.0216 (8) |
| O2 | 0.0509 (6) | 0.1051 (9) | 0.0568 (7) | −0.0042 (6) | −0.0083 (5) | −0.0022 (6) |
| C1 | 0.0433 (7) | 0.0458 (7) | 0.0447 (8) | −0.0016 (5) | 0.0056 (5) | 0.0043 (5) |
| C2 | 0.0471 (8) | 0.0500 (8) | 0.0498 (8) | −0.0030 (6) | −0.0009 (6) | 0.0033 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C3 | 0.0680 (10) | 0.0567 (8) | 0.0457 (8) | 0.0016 (7) | 0.0013 (7) | −0.0087 (6) |
| C4 | 0.0613 (9) | 0.0534 (8) | 0.0555 (9) | 0.0088 (6) | 0.0156 (7) | −0.0047 (6) |
| C5 | 0.0475 (7) | 0.0399 (7) | 0.0533 (8) | 0.0015 (5) | 0.0082 (6) | 0.0027 (6) |
| C6 | 0.0469 (8) | 0.0604 (9) | 0.0727 (11) | 0.0051 (6) | 0.0122 (7) | 0.0066 (7) |
| C7 | 0.0431 (8) | 0.0705 (10) | 0.0782 (12) | −0.0019 (7) | −0.0039 (7) | 0.0090 (8) |
| C8 | 0.0575 (9) | 0.0658 (9) | 0.0595 (10) | −0.0065 (7) | −0.0090 (7) | −0.0017 (7) |
| C9 | 0.0523 (8) | 0.0546 (8) | 0.0508 (8) | −0.0024 (6) | 0.0028 (6) | −0.0024 (6) |
| C10 | 0.0453 (7) | 0.0372 (6) | 0.0456 (8) | −0.0018 (5) | 0.0045 (5) | 0.0035 (5) |
| C11 | 0.0463 (8) | 0.0847 (11) | 0.0552 (9) | 0.0004 (7) | 0.0089 (6) | 0.0020 (8) |
| C12 | 0.0713 (11) | 0.1163 (16) | 0.0632 (11) | −0.0073 (10) | −0.0195 (9) | −0.0018 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C11 | 1.1991 (18) | C6—C7 | 1.357 (2) |
| O2—C2 | 1.3615 (16) | C6—H6 | 0.93 |
| O2—C12 | 1.4180 (19) | C7—C8 | 1.393 (2) |
| C1—C2 | 1.3877 (19) | C7—H7 | 0.93 |
| C1—C10 | 1.4336 (18) | C8—C9 | 1.364 (2) |
| C1—C11 | 1.4641 (19) | C8—H8 | 0.93 |
| C2—C3 | 1.405 (2) | C9—C10 | 1.4137 (19) |
| C3—C4 | 1.354 (2) | C9—H9 | 0.93 |
| C3—H3 | 0.93 | C11—H11 | 0.93 |
| C4—C5 | 1.409 (2) | C12—H12A | 0.96 |
| C4—H4 | 0.93 | C12—H12B | 0.96 |
| C5—C6 | 1.414 (2) | C12—H12C | 0.96 |
| C5—C10 | 1.4219 (19) | | |
| C2—O2—C12 | 119.74 (13) | C6—C7—H7 | 120.1 |
| C2—C1—C10 | 119.47 (12) | C8—C7—H7 | 120.1 |
| C2—C1—C11 | 117.16 (12) | C9—C8—C7 | 121.22 (14) |
| C10—C1—C11 | 123.34 (12) | C9—C8—H8 | 119.4 |
| O2—C2—C1 | 116.27 (12) | C7—C8—H8 | 119.4 |
| O2—C2—C3 | 122.61 (13) | C8—C9—C10 | 120.94 (14) |
| C1—C2—C3 | 121.11 (13) | C8—C9—H9 | 119.5 |
| C4—C3—C2 | 119.60 (13) | C10—C9—H9 | 119.5 |
| C4—C3—H3 | 120.2 | C9—C10—C5 | 117.58 (12) |
| C2—C3—H3 | 120.2 | C9—C10—C1 | 123.75 (12) |
| C3—C4—C5 | 122.21 (13) | C5—C10—C1 | 118.67 (12) |
| C3—C4—H4 | 118.9 | O1—C11—C1 | 127.75 (15) |
| C5—C4—H4 | 118.9 | O1—C11—H11 | 116.1 |
| C4—C5—C6 | 121.50 (13) | C1—C11—H11 | 116.1 |
| C4—C5—C10 | 118.91 (13) | O2—C12—H12A | 109.5 |
| C6—C5—C10 | 119.59 (13) | O2—C12—H12B | 109.5 |
| C7—C6—C5 | 120.87 (14) | H12A—C12—H12B | 109.5 |
| C7—C6—H6 | 119.6 | O2—C12—H12C | 109.5 |
| C5—C6—H6 | 119.6 | H12A—C12—H12C | 109.5 |
| C6—C7—C8 | 119.79 (14) | H12B—C12—H12C | 109.5 |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12C···O1$^{i}$ | 0.96 | 2.46 | 3.362 (4) | 156 (6) |

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

**Fig. 1**

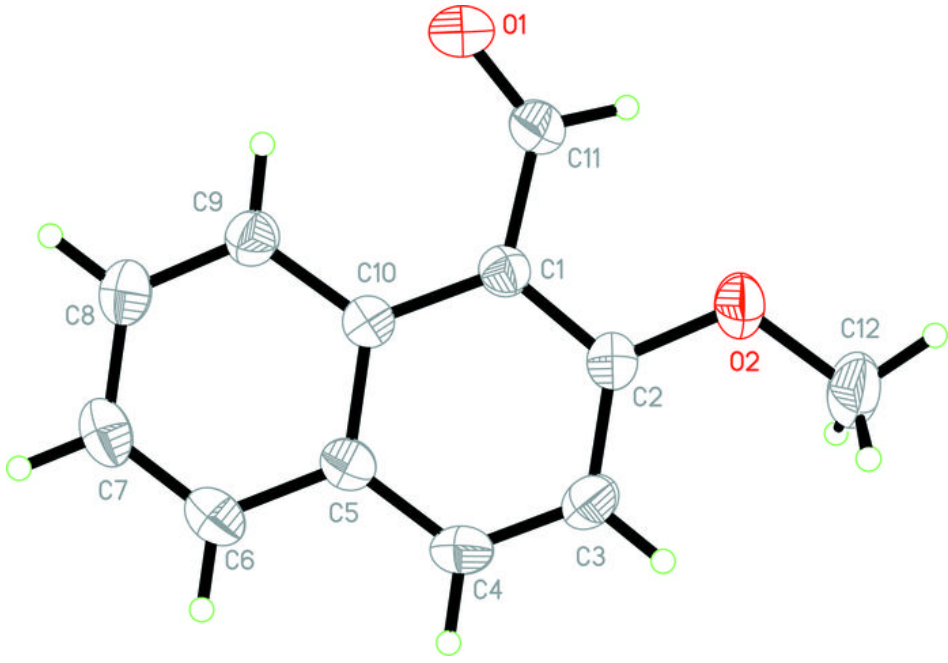

**Fig. 2**