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## Structure Reports

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## 2-Methoxynaphthalene-1-carbaldehyde

Chunbao Tang

Department of Chemistry, Jiaying University, Meizhou 514015, People's Republic of China

Correspondence e-mail: chunbao\_tang@126.com

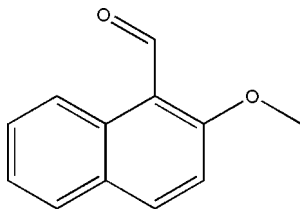
Received 15 April 2009; accepted 16 April 2009

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

In the title compound,  $\text{C}_{12}\text{H}_{10}\text{O}_2$ , 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  $\text{C}-\text{H}\cdots\text{O}$  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

$\text{C}_{12}\text{H}_{10}\text{O}_2$   
 $M_r = 186.20$   
 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<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation

$\mu = 0.09$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.20 \times 0.20 \times 0.18$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.018$

## 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  
 $\Delta\rho_{\text{max}} = 0.12$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.17$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C12}-\text{H12C}\cdots\text{O1}^i$	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.

Financial support from the Jiaying University Research Fund is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2783).

## References

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## supporting information

*Acta Cryst.* (2009). E65, o1088 [doi:10.1107/S1600536809014287]

## 2-Methoxynaphthalene-1-carbaldehyde

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### S1. 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)°].

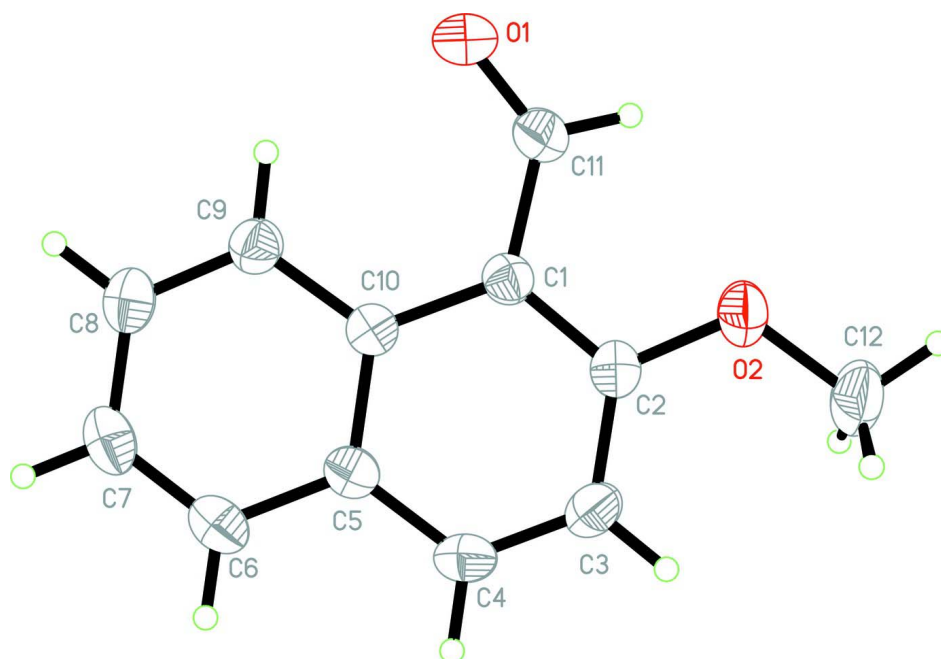
In the crystal structure, molecules are linked through intermolecular C—H···O hydrogen bonds (Table 1), forming chains running along the *c* axis (Fig. 2).

### S2. Experimental

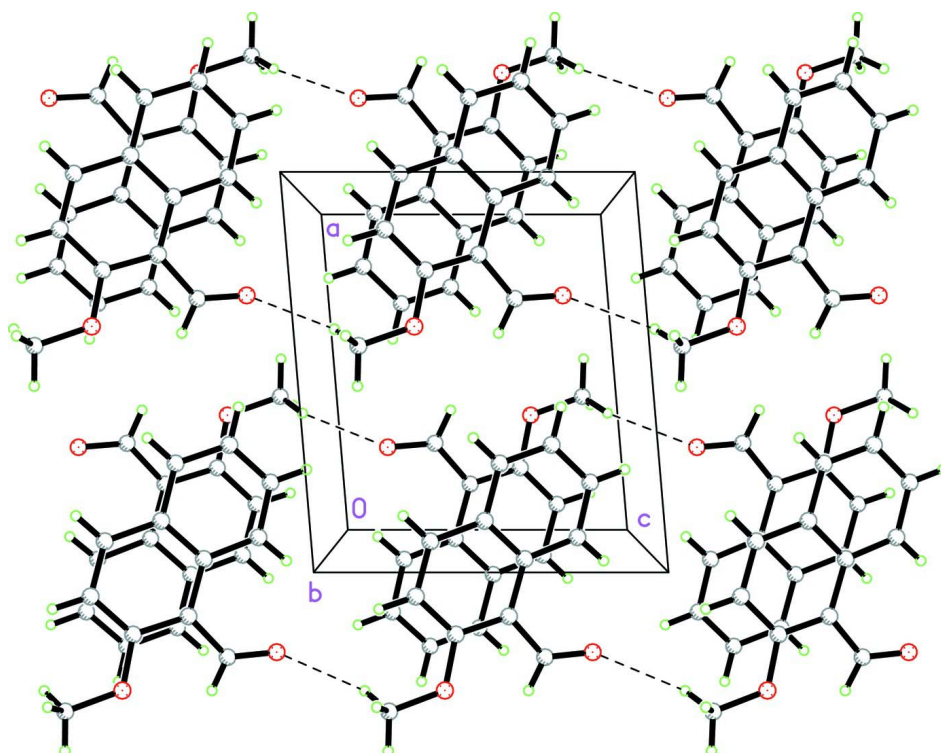
The title compound was obtained commercially (Lancaster). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution of the compound.

### S3. Refinement

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

**Figure 1**

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

**Figure 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<sub>12</sub>H<sub>10</sub>O<sub>2</sub> $M_r = 186.20$ Monoclinic,  $P2_1/c$ 

Hall symbol: -P 2ybc

 $a = 8.689$  (3) Å $b = 14.155$  (4) Å $c = 7.667$  (2) Å $\beta = 94.805$  (4)° $V = 939.7$  (5) Å<sup>3</sup> $Z = 4$  $F(000) = 392$  $D_x = 1.316$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1550 reflections

 $\theta = 2.3$ – $25.3$ ° $\mu = 0.09$  mm<sup>-1</sup> $T = 298$  K

Block, colourless

 $0.20 \times 0.20 \times 0.18$  mm

## Data collection

Bruker SMART CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\omega$  scansAbsorption correction: multi-scan  
(*SADABS*; Sheldrick, 1996) $T_{\min} = 0.982$ ,  $T_{\max} = 0.984$ 

5187 measured reflections

2046 independent reflections

1477 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.018$  $\theta_{\text{max}} = 27.0$ °,  $\theta_{\text{min}} = 2.4$ ° $h = -8 \rightarrow 11$  $k = -17 \rightarrow 18$  $l = -8 \rightarrow 9$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.043$  $wR(F^2) = 0.124$  $S = 1.03$ 

2046 reflections

128 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.1007P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} = 0.001$  $\Delta\rho_{\text{max}} = 0.12$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.17$  e Å<sup>-3</sup>

## 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<sup>2</sup>)

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
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<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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)		
<hr/>			
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, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C12—H12C...O1 <sup>i</sup>	0.96	2.46	3.362 (4)	156 (6)

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