Acta Cryst E STRUCTURE REPORTS

OPEN ACCESS

ISSN 1600-5368

# Crystal structure of 4-methoxy-*N*-phenylbenzamide

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Received 14 July 2014; accepted 15 July 2014

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

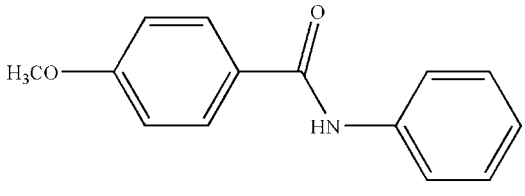
In the title molecule, $C_{14}H_{13}NO_2$, the dihedral angle between the planes of the benzene rings is 65.18 (4)°. The central amide group has about the same degree of twist with respect to both ring planes, as indicated by the dihedral angles of 34.70 (8) and 30.62 (8)° between its plane and that of the phenyl and 4-methoxybenzene rings, respectively. The C atom of the methoxy group is close to being coplanar with its attached ring [deviation = −0.112 (2) Å]. In the crystal, molecules are linked by inter-amide N—H···O hydrogen bonds, which generate *C*(4) chains propagating in the [100] direction. Adajcent molecules in the chain are related by translational symmetry.

**Keywords:** crystal structure; amide; *C*(4) chain; hydrogen bonding.

**CCDC reference**: 1014108

## 1. Related literature

The background to this work has been described in earlier papers; see: Ren *et al.* (2010); Zhu *et al.* (2011). For related structures, see: Raza *et al.* (2010); Gowda *et al.* (2003).




## 2. Experimental

### 2.1. Crystal data

$C_{14}H_{13}NO_2$ $M_r$ = 227.25

Triclinic, $P\overline{1}$
$a$ = 5.308 (3) Å
$b$ = 7.709 (4) Å
$c$ = 14.109 (7) Å
$\alpha$ = 96.911 (8)°
$\beta$ = 99.210 (8)°
$\gamma$ = 90.511 (9)°
$V$ = 565.5 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
0.30 × 0.20 × 0.20 mm

### 2.2. Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.974, $T_{max}$ = 0.982
3188 measured reflections
2005 independent reflections
1605 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.013

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
$S$ = 1.03
2005 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 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···$A$ |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.86 | 2.31 | 3.110 (2) | 154 |

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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* and *PLATON* (Spek, 2009).

## Acknowledgements

We gratefully acknowledge the Natural Science Foundation of China (grant No. 21201024), the Natural Science Foundation of Shanxi province (grant No. 2012021009-1) and the College Student's Innovation Traning Project in Shanxi Province (grant No. 2013319).

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7253).

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# supporting information

*Acta Cryst.* (2014). E**70**, o921 [doi:10.1107/S1600536814016420]

## Crystal structure of 4-methoxy-*N*-phenylbenzamide

**Zhijun Wang, Haiying Lei, Linhua Jin and Ruitao Zhu**

### S1. Experimental

To a 100 ml round flask fitted with a condenser was added aniline (0.93 g, 10 mmol), dichloromethane (15 ml) and triethylamine(0.5 ml) with magnetic stirring. 4-methoxybenzoyl chloride (1.70 g, 10 mmol) was added gradually. The reaction mixture was stirred at room temperature for 1 h and then refluxed for 2 h. The product precipitated as a white powder, which was washed three times with water and dichloromethane. Recrystallization from ethyl alcohol solution produced colourless prisms of the title compound.

### S2. Refinement

H atoms were placed in idealized positions and allowed to ride on their respective parent atoms, with C—H = 0.93 Å, N—H = 0.86 Å and $U_{iso}$(H)= 1.2$U_{eq}$(C,*N*).

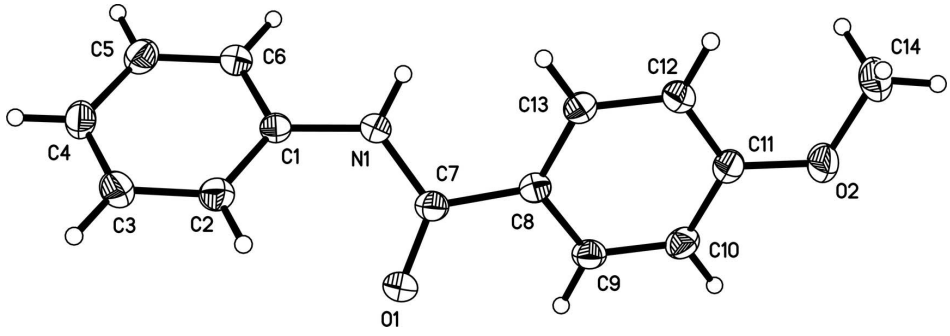


**Figure 1**

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

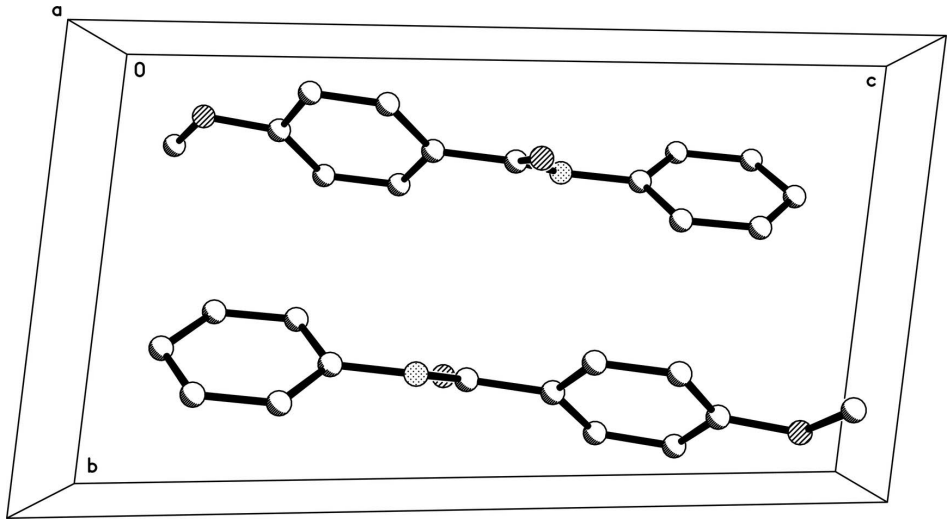


**Figure 2**

Part of the crystal structure of (I) with the donor-acceptor distances of hydrogen bonds drawn as dashed lines. H atoms are not shown.

### 4-Methoxy-*N*-phenylbenzamide

*Crystal data*

$C_{14}H_{13}NO_2$
$M_r = 227.25$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.308$ (3) Å
$b = 7.709$ (4) Å
$c = 14.109$ (7) Å
$\alpha = 96.911$ (8)°
$\beta = 99.210$ (8)°
$\gamma = 90.511$ (9)°
$V = 565.5$ (5) Å$^3$
$Z = 2$
$F(000) = 240$
$D_x = 1.335$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\theta = 1.5$–$25.1$°
$\mu = 0.09$ mm$^{-1}$
$T = 296$ K
Prism, colorless
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.974$, $T_{max} = 0.982$
3188 measured reflections
2005 independent reflections
1605 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 25.1°$, $\theta_{min} = 1.5°$
$h = -5 \rightarrow 6$
$k = -8 \rightarrow 9$
$l = -16 \rightarrow 16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.097$
$S = 1.03$
2005 reflections
156 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

$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.1154P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å$^{-3}$
$\Delta\rho_{min} = -0.13$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.037 (5)

*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 | 0.2321 (2) | 0.27538 (17) | 0.57341 (8) | 0.0387 (3) |
| H1 | 0.0748 | 0.2753 | 0.5465 | 0.046* |
| O1 | 0.63875 (19) | 0.25639 (17) | 0.54382 (8) | 0.0542 (4) |
| O2 | 0.0921 (2) | 0.14685 (16) | 0.11034 (7) | 0.0520 (3) |
| C1 | 0.2818 (3) | 0.29568 (19) | 0.67586 (10) | 0.0340 (3) |
| C2 | 0.4919 (3) | 0.3893 (2) | 0.72863 (11) | 0.0427 (4) |
| H2 | 0.6085 | 0.4409 | 0.6971 | 0.051* |
| C3 | 0.5279 (3) | 0.4060 (2) | 0.82849 (12) | 0.0504 (4) |
| H3 | 0.6693 | 0.4693 | 0.8638 | 0.060* |
| C4 | 0.3582 (3) | 0.3307 (2) | 0.87637 (11) | 0.0483 (4) |
| H4 | 0.3849 | 0.3414 | 0.9436 | 0.058* |
| C5 | 0.1478 (3) | 0.2391 (2) | 0.82331 (11) | 0.0468 (4) |
| H5 | 0.0306 | 0.1889 | 0.8551 | 0.056* |
| C6 | 0.1091 (3) | 0.2210 (2) | 0.72366 (11) | 0.0401 (4) |
| H6 | −0.0333 | 0.1585 | 0.6886 | 0.048* |
| C7 | 0.4093 (3) | 0.2561 (2) | 0.51365 (11) | 0.0373 (4) |
| C8 | 0.3083 (3) | 0.22995 (19) | 0.40820 (10) | 0.0345 (3) |
| C9 | 0.4522 (3) | 0.1323 (2) | 0.34765 (11) | 0.0390 (4) |
| H9 | 0.6042 | 0.0850 | 0.3742 | 0.047* |
| C10 | 0.3727 (3) | 0.1051 (2) | 0.24959 (11) | 0.0415 (4) |
| H10 | 0.4676 | 0.0365 | 0.2103 | 0.050* |
| C11 | 0.1516 (3) | 0.1795 (2) | 0.20900 (10) | 0.0377 (4) |
| C12 | 0.0070 (3) | 0.2788 (2) | 0.26739 (11) | 0.0395 (4) |
| H12 | −0.1412 | 0.3297 | 0.2403 | 0.047* |
| C13 | 0.0852 (3) | 0.3014 (2) | 0.36659 (10) | 0.0378 (4) |
| H13 | −0.0139 | 0.3658 | 0.4060 | 0.045* |
| C14 | −0.1445 (4) | 0.2052 (3) | 0.06486 (12) | 0.0631 (5) |
| H14A | −0.2804 | 0.1623 | 0.0940 | 0.095* |
| H14B | −0.1707 | 0.1620 | −0.0028 | 0.095* |
| H14C | −0.1425 | 0.3307 | 0.0726 | 0.095* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0288 (6) | 0.0535 (8) | 0.0333 (7) | 0.0023 (5) | 0.0034 (5) | 0.0053 (6) |
| O1 | 0.0299 (6) | 0.0892 (10) | 0.0424 (7) | 0.0060 (6) | 0.0046 (5) | 0.0050 (6) |
| O2 | 0.0563 (7) | 0.0653 (8) | 0.0327 (6) | 0.0104 (6) | 0.0067 (5) | 0.0000 (5) |
| C1 | 0.0313 (7) | 0.0364 (8) | 0.0342 (8) | 0.0065 (6) | 0.0052 (6) | 0.0035 (6) |
| C2 | 0.0360 (8) | 0.0479 (10) | 0.0434 (9) | −0.0027 (7) | 0.0083 (7) | −0.0002 (7) |
| C3 | 0.0418 (9) | 0.0583 (11) | 0.0453 (10) | 0.0005 (8) | 0.0001 (7) | −0.0073 (8) |
| C4 | 0.0520 (10) | 0.0587 (11) | 0.0325 (8) | 0.0115 (8) | 0.0045 (7) | 0.0016 (7) |
| C5 | 0.0471 (9) | 0.0546 (11) | 0.0418 (9) | 0.0046 (8) | 0.0140 (7) | 0.0088 (8) |
| C6 | 0.0333 (8) | 0.0477 (9) | 0.0387 (8) | −0.0004 (7) | 0.0055 (6) | 0.0036 (7) |
| C7 | 0.0309 (8) | 0.0416 (9) | 0.0399 (8) | 0.0030 (6) | 0.0059 (6) | 0.0066 (7) |
| C8 | 0.0314 (7) | 0.0370 (8) | 0.0358 (8) | −0.0006 (6) | 0.0072 (6) | 0.0051 (6) |
| C9 | 0.0313 (8) | 0.0427 (9) | 0.0437 (9) | 0.0050 (6) | 0.0072 (6) | 0.0059 (7) |
| C10 | 0.0400 (8) | 0.0446 (9) | 0.0411 (9) | 0.0060 (7) | 0.0142 (7) | −0.0004 (7) |
| C11 | 0.0403 (8) | 0.0390 (9) | 0.0343 (8) | −0.0009 (7) | 0.0087 (6) | 0.0033 (6) |
| C12 | 0.0348 (8) | 0.0451 (9) | 0.0379 (8) | 0.0062 (7) | 0.0035 (6) | 0.0052 (7) |
| C13 | 0.0357 (8) | 0.0408 (9) | 0.0372 (8) | 0.0062 (6) | 0.0094 (6) | 0.0010 (7) |
| C14 | 0.0676 (12) | 0.0819 (14) | 0.0369 (9) | 0.0150 (10) | 0.0004 (8) | 0.0059 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C7 | 1.3580 (19) | C6—H6 | 0.9300 |
| N1—C1 | 1.4164 (19) | C7—C8 | 1.487 (2) |
| N1—H1 | 0.8600 | C8—C13 | 1.385 (2) |
| O1—C7 | 1.2242 (18) | C8—C9 | 1.394 (2) |
| O2—C11 | 1.3689 (18) | C9—C10 | 1.370 (2) |
| O2—C14 | 1.419 (2) | C9—H9 | 0.9300 |
| C1—C2 | 1.382 (2) | C10—C11 | 1.382 (2) |
| C1—C6 | 1.381 (2) | C10—H10 | 0.9300 |
| C2—C3 | 1.381 (2) | C11—C12 | 1.384 (2) |
| C2—H2 | 0.9300 | C12—C13 | 1.384 (2) |
| C3—C4 | 1.373 (2) | C12—H12 | 0.9300 |
| C3—H3 | 0.9300 | C13—H13 | 0.9300 |
| C4—C5 | 1.378 (2) | C14—H14A | 0.9600 |
| C4—H4 | 0.9300 | C14—H14B | 0.9600 |
| C5—C6 | 1.378 (2) | C14—H14C | 0.9600 |
| C5—H5 | 0.9300 | | |
| | | | |
| C7—N1—C1 | 126.16 (12) | C13—C8—C9 | 118.33 (14) |
| C7—N1—H1 | 116.9 | C13—C8—C7 | 123.93 (13) |
| C1—N1—H1 | 116.9 | C9—C8—C7 | 117.71 (13) |
| C11—O2—C14 | 118.22 (13) | C10—C9—C8 | 120.86 (14) |
| C2—C1—C6 | 119.58 (14) | C10—C9—H9 | 119.6 |
| C2—C1—N1 | 122.48 (13) | C8—C9—H9 | 119.6 |
| C6—C1—N1 | 117.92 (13) | C9—C10—C11 | 120.12 (14) |
| C1—C2—C3 | 119.65 (15) | C9—C10—H10 | 119.9 |

| | | | |
|---|---|---|---|
| C1—C2—H2 | 120.2 | C11—C10—H10 | 119.9 |
| C3—C2—H2 | 120.2 | O2—C11—C10 | 115.38 (13) |
| C4—C3—C2 | 121.03 (16) | O2—C11—C12 | 124.49 (14) |
| C4—C3—H3 | 119.5 | C10—C11—C12 | 120.13 (14) |
| C2—C3—H3 | 119.5 | C13—C12—C11 | 119.30 (14) |
| C3—C4—C5 | 119.01 (15) | C13—C12—H12 | 120.4 |
| C3—C4—H4 | 120.5 | C11—C12—H12 | 120.4 |
| C5—C4—H4 | 120.5 | C12—C13—C8 | 121.22 (14) |
| C4—C5—C6 | 120.70 (15) | C12—C13—H13 | 119.4 |
| C4—C5—H5 | 119.6 | C8—C13—H13 | 119.4 |
| C6—C5—H5 | 119.6 | O2—C14—H14A | 109.5 |
| C5—C6—C1 | 120.02 (15) | O2—C14—H14B | 109.5 |
| C5—C6—H6 | 120.0 | H14A—C14—H14B | 109.5 |
| C1—C6—H6 | 120.0 | O2—C14—H14C | 109.5 |
| O1—C7—N1 | 122.62 (14) | H14A—C14—H14C | 109.5 |
| O1—C7—C8 | 121.34 (13) | H14B—C14—H14C | 109.5 |
| N1—C7—C8 | 116.02 (13) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.86 | 2.31 | 3.110 (2) | 154 |

Symmetry code: (i) *x*−1, *y*, *z*.