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# 2-Methyl-*N*-(3-methylphenyl)benzamide

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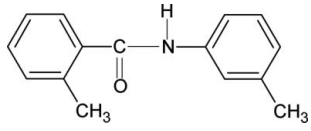
Key indicators: single-crystal X-ray study; $T$ = 299 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.037; $wR$ factor = 0.101; data-to-parameter ratio = 7.4.

In the structure of the title compound (N3MP2MBA), $C_{15}H_{15}NO$, the conformation of the N—H bond is *anti* to the *meta*-methyl substituent in the aniline ring and that of the C═O bond is *syn* to the *ortho*-methyl substituent in the benzoyl ring, while the conformations of the N—H and C═O bonds are *anti* to each other. The bond parameters in N3MP2MBA are similar to those in 2-methyl-*N*-phenylbenzamide, *N*-(3,4-dimethylphenyl)benzamide and other benzanilides. The amide group, –NHCO–, makes a dihedral angle of 55.2 (7)° with the benzoyl ring, while the dihedral angle between the two benzene rings (benzoyl and aniline) is 36.2 (1)°. N—H···O hydrogen bonds give rise to infinite chains running along the *b* axis of the crystal structure.

## Related literature

For related literature, see: Gowda *et al.* (2003; 2008*a*,*b*).




## Experimental

### Crystal data

$C_{15}H_{15}NO$
$M_r$ = 225.28
Tetragonal, $P4_3$
$a$ = 8.931 (2) Å
$c$ = 15.816 (4) Å
$V$ = 1261.5 (3) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 0.58 mm$^{-1}$
$T$ = 299 (2) K
0.55 × 0.30 × 0.30 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
1606 measured reflections
1168 independent reflections
1096 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.100
$S$ = 1.07
1168 reflections
158 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.12 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.10 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*···O1$^{i}$ | 0.837 (18) | 2.10 (2) | 2.908 (3) | 163 (3) |

Symmetry code: (i) $-y+1, x, z-\frac{1}{4}$.

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

BTG thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2212).

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# supporting information

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## 2-Methyl-*N*-(3-methylphenyl)benzamide

**B. Thimme Gowda, Sabine Foro, B. P. Sowmya and Hartmut Fuess**

### S1. Comment

As part of a study of the substituent effects on the structures of N-aromatic amides, in the present work, the structure of *N*-(3-methylphenyl)-2-methylbenzamide (N3MP2MBA) has been determined (Gowda *et al.*, 2003; 2008*a*; 2008*b*). In the structure of N3MP2MBA (Fig. 1), the conformation of the N—H bond is *anti* to the *meta*-methyl substituent in the aniline ring and that of the C=O bond is *syn* to the *ortho*-methyl substituent in the benzoyl ring, while the conformations of the N—H and C=O bonds are *anti* to each other. The bond parameters in N2MP2MBA are similar to those in *N*-(phenyl)-2-methylbenzamide (Gowda *et al.*, 2008*a*), *N*-(3,4-dimethylphenyl)-benzamide (Gowda *et al.*, 2008*b*) and other benzanilides (Gowda *et al.*, 2003). The amide group –NHCO– has the dihedral angle of 55.2 (7)° with the benzoyl ring, while the dihedral angle between the two benzene rings (benzoyl and aniline) is 36.2 (1)°. The packing diagram of N3MP2MBA molecules showing the hydrogen bonds N1—H1N···O1 (Table 1) involved in the formation of molecular chain is given in Fig. 2.

### S2. Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra. Single crystals of the title compound were obtained from an ethanolic solution and used for X-ray diffraction studies at room temperature.

### S3. Refinement

The NH atom was located in difference map and was refined with restrained geometry, *viz*. N—H distance was restrained to 0.86 (2) Å. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93–0.96 Å A l l H atoms were refined with isotropic displacement parameters (set to 1.2 times of the $U_{eq}$ of the parent atom).

In the absence of significant anomalous dispersion effects, Friedel pairs were merged and the Δf''term set to zero.

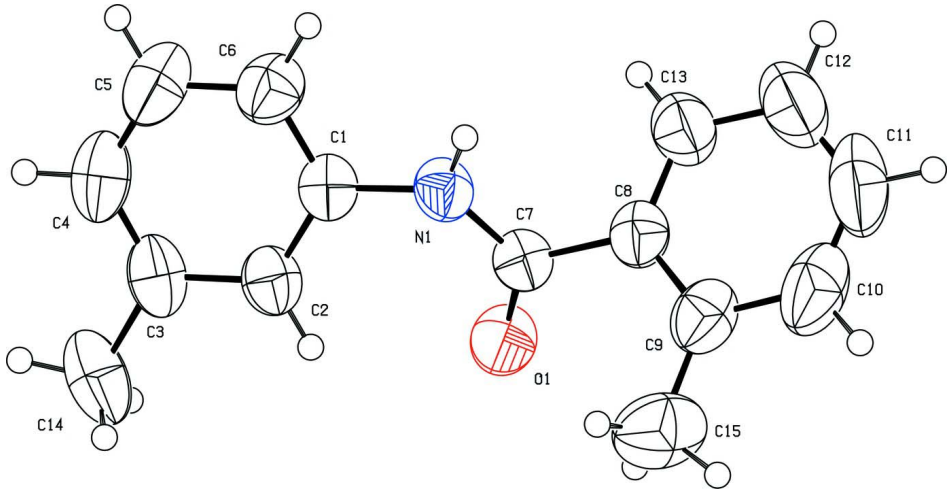


**Figure 1**

Molecular structure of the title compound, showing the atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level.

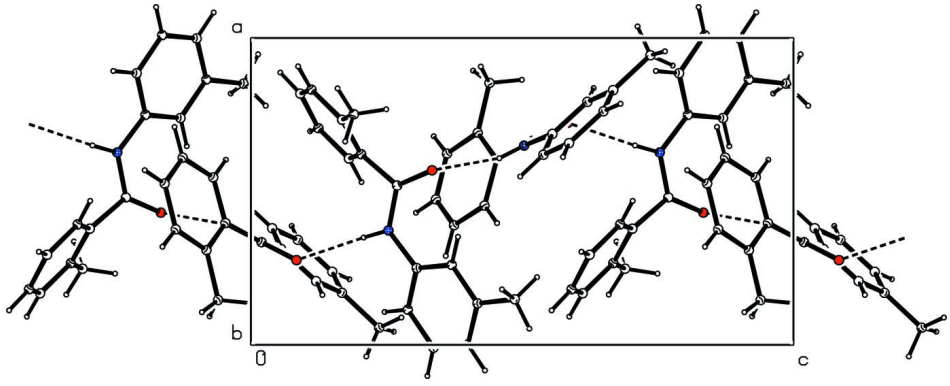


**Figure 2**

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

### 2-Methyl-*N*-(3-methylphenyl)benzamide

*Crystal data*

$C_{15}H_{15}NO$
$M_r = 225.28$
Tetragonal, $P4_3$
Hall symbol: P 4cw
$a = 8.931$ (2) Å
$c = 15.816$ (4) Å
$V = 1261.5$ (3) Å$^3$
$Z = 4$
$F(000) = 480$
$D_x = 1.186$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 4.9$–$19.0°$
$\mu = 0.58$ mm$^{-1}$
$T = 299$ K
Prism, colourless
0.55 × 0.30 × 0.30 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
1606 measured reflections
1168 independent reflections
1096 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.016
$\theta_{max}$ = 66.8°, $\theta_{min}$ = 5.0°
$h$ = −10→0
$k$ = −10→0
$l$ = −18→3
3 standard reflections every 120 min
intensity decay: 1.0%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.100
$S$ = 1.07
1168 reflections
158 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.0805P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.10 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0069 (14)

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.3124 (3) | 0.2503 (2) | 0.05561 (14) | 0.0534 (5) |
| C2 | 0.2079 (3) | 0.2607 (3) | 0.12012 (15) | 0.0601 (6) |
| H2 | 0.1629 | 0.3523 | 0.1317 | 0.072* |
| C3 | 0.1696 (3) | 0.1353 (3) | 0.16775 (15) | 0.0681 (7) |
| C4 | 0.2385 (4) | 0.0013 (3) | 0.1499 (2) | 0.0827 (9) |
| H4 | 0.2142 | −0.0833 | 0.1813 | 0.099* |
| C5 | 0.3424 (4) | −0.0095 (3) | 0.0865 (2) | 0.0874 (9) |
| H5 | 0.3877 | −0.1011 | 0.0752 | 0.105* |
| C6 | 0.3802 (3) | 0.1149 (3) | 0.03921 (17) | 0.0718 (7) |
| H6 | 0.4512 | 0.1072 | −0.0036 | 0.086* |
| C7 | 0.3347 (2) | 0.5195 (2) | 0.01949 (14) | 0.0521 (5) |
| C8 | 0.3969 (3) | 0.6215 (3) | −0.04697 (15) | 0.0576 (6) |
| C9 | 0.3085 (4) | 0.7335 (3) | −0.08194 (17) | 0.0729 (7) |
| C10 | 0.3766 (6) | 0.8318 (4) | −0.1386 (2) | 0.1034 (12) |
| H10 | 0.3200 | 0.9078 | −0.1630 | 0.124* |
| C11 | 0.5257 (7) | 0.8189 (4) | −0.1590 (3) | 0.1172 (16) |
| H11A | 0.5692 | 0.8874 | −0.1958 | 0.141* |
| C12 | 0.6101 (5) | 0.7064 (5) | −0.1257 (3) | 0.1091 (13) |
| H12A | 0.7102 | 0.6964 | −0.1408 | 0.131* |

| | | | | |
|---|---|---|---|---|
| C13 | 0.5459 (4) | 0.6074 (3) | −0.0694 (2) | 0.0774 (8) |
| H13 | 0.6033 | 0.5307 | −0.0463 | 0.093* |
| C14 | 0.0560 (4) | 0.1486 (5) | 0.2363 (2) | 0.0956 (10) |
| H14A | −0.0376 | 0.1807 | 0.2127 | 0.115* |
| H14B | 0.0894 | 0.2206 | 0.2773 | 0.115* |
| H14C | 0.0431 | 0.0531 | 0.2632 | 0.115* |
| C15 | 0.1464 (4) | 0.7517 (5) | −0.0604 (3) | 0.1053 (12) |
| H15A | 0.1361 | 0.7678 | −0.0007 | 0.126* |
| H15B | 0.0928 | 0.6629 | −0.0763 | 0.126* |
| H15C | 0.1064 | 0.8361 | −0.0904 | 0.126* |
| N1 | 0.3505 (2) | 0.3731 (2) | 0.00353 (13) | 0.0561 (5) |
| H1N | 0.392 (3) | 0.350 (3) | −0.0422 (14) | 0.067* |
| O1 | 0.2763 (2) | 0.56893 (19) | 0.08395 (11) | 0.0681 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0613 (12) | 0.0547 (12) | 0.0444 (11) | −0.0074 (9) | −0.0062 (10) | −0.0018 (9) |
| C2 | 0.0662 (13) | 0.0625 (13) | 0.0515 (13) | −0.0094 (10) | −0.0007 (11) | 0.0011 (11) |
| C3 | 0.0790 (16) | 0.0749 (16) | 0.0504 (14) | −0.0251 (13) | −0.0092 (12) | 0.0083 (12) |
| C4 | 0.112 (2) | 0.0683 (16) | 0.0680 (17) | −0.0192 (15) | −0.0136 (17) | 0.0189 (14) |
| C5 | 0.123 (2) | 0.0562 (14) | 0.083 (2) | 0.0044 (15) | −0.007 (2) | 0.0070 (15) |
| C6 | 0.0897 (18) | 0.0639 (14) | 0.0619 (16) | 0.0042 (12) | 0.0023 (14) | −0.0021 (12) |
| C7 | 0.0558 (11) | 0.0558 (11) | 0.0447 (11) | −0.0033 (9) | −0.0023 (9) | −0.0026 (9) |
| C8 | 0.0721 (14) | 0.0517 (12) | 0.0490 (12) | −0.0063 (10) | 0.0031 (11) | −0.0049 (10) |
| C9 | 0.102 (2) | 0.0610 (14) | 0.0560 (15) | 0.0059 (13) | −0.0007 (14) | 0.0014 (12) |
| C10 | 0.173 (4) | 0.0676 (17) | 0.070 (2) | 0.008 (2) | 0.016 (2) | 0.0166 (15) |
| C11 | 0.180 (4) | 0.078 (2) | 0.093 (3) | −0.043 (3) | 0.047 (3) | 0.003 (2) |
| C12 | 0.111 (3) | 0.093 (2) | 0.123 (3) | −0.033 (2) | 0.047 (3) | −0.007 (2) |
| C13 | 0.0777 (17) | 0.0716 (16) | 0.0828 (19) | −0.0131 (13) | 0.0141 (15) | −0.0023 (14) |
| C14 | 0.107 (2) | 0.112 (2) | 0.0678 (18) | −0.0414 (19) | 0.0137 (18) | 0.0095 (18) |
| C15 | 0.105 (3) | 0.125 (3) | 0.086 (2) | 0.038 (2) | −0.011 (2) | 0.012 (2) |
| N1 | 0.0679 (12) | 0.0564 (10) | 0.0440 (9) | −0.0042 (8) | 0.0088 (9) | −0.0027 (8) |
| O1 | 0.0946 (12) | 0.0628 (10) | 0.0468 (9) | 0.0015 (9) | 0.0096 (9) | −0.0054 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.377 (4) | C9—C10 | 1.394 (5) |
| C1—C2 | 1.386 (3) | C9—C15 | 1.496 (5) |
| C1—N1 | 1.414 (3) | C10—C11 | 1.375 (7) |
| C2—C3 | 1.392 (3) | C10—H10 | 0.9300 |
| C2—H2 | 0.9300 | C11—C12 | 1.361 (7) |
| C3—C4 | 1.375 (5) | C11—H11A | 0.9300 |
| C3—C14 | 1.490 (5) | C12—C13 | 1.380 (5) |
| C4—C5 | 1.369 (5) | C12—H12A | 0.9300 |
| C4—H4 | 0.9300 | C13—H13 | 0.9300 |
| C5—C6 | 1.381 (4) | C14—H14A | 0.9600 |
| C5—H5 | 0.9300 | C14—H14B | 0.9600 |

| | | | |
|---|---|---|---|
| C6—H6 | 0.9300 | C14—H14C | 0.9600 |
| C7—O1 | 1.227 (3) | C15—H15A | 0.9600 |
| C7—N1 | 1.339 (3) | C15—H15B | 0.9600 |
| C7—C8 | 1.498 (3) | C15—H15C | 0.9600 |
| C8—C13 | 1.382 (4) | N1—H1N | 0.837 (18) |
| C8—C9 | 1.389 (4) | | |

| | | | |
|---|---|---|---|
| C6—C1—C2 | 119.6 (2) | C11—C10—C9 | 121.4 (4) |
| C6—C1—N1 | 117.8 (2) | C11—C10—H10 | 119.3 |
| C2—C1—N1 | 122.6 (2) | C9—C10—H10 | 119.3 |
| C1—C2—C3 | 120.6 (2) | C12—C11—C10 | 120.5 (3) |
| C1—C2—H2 | 119.7 | C12—C11—H11A | 119.8 |
| C3—C2—H2 | 119.7 | C10—C11—H11A | 119.8 |
| C4—C3—C2 | 118.6 (3) | C11—C12—C13 | 119.5 (4) |
| C4—C3—C14 | 121.6 (3) | C11—C12—H12A | 120.2 |
| C2—C3—C14 | 119.8 (3) | C13—C12—H12A | 120.2 |
| C5—C4—C3 | 121.0 (3) | C12—C13—C8 | 120.4 (3) |
| C5—C4—H4 | 119.5 | C12—C13—H13 | 119.8 |
| C3—C4—H4 | 119.5 | C8—C13—H13 | 119.8 |
| C4—C5—C6 | 120.4 (3) | C3—C14—H14A | 109.5 |
| C4—C5—H5 | 119.8 | C3—C14—H14B | 109.5 |
| C6—C5—H5 | 119.8 | H14A—C14—H14B | 109.5 |
| C1—C6—C5 | 119.8 (3) | C3—C14—H14C | 109.5 |
| C1—C6—H6 | 120.1 | H14A—C14—H14C | 109.5 |
| C5—C6—H6 | 120.1 | H14B—C14—H14C | 109.5 |
| O1—C7—N1 | 123.5 (2) | C9—C15—H15A | 109.5 |
| O1—C7—C8 | 121.5 (2) | C9—C15—H15B | 109.5 |
| N1—C7—C8 | 114.97 (19) | H15A—C15—H15B | 109.5 |
| C13—C8—C9 | 120.7 (3) | C9—C15—H15C | 109.5 |
| C13—C8—C7 | 118.8 (2) | H15A—C15—H15C | 109.5 |
| C9—C8—C7 | 120.4 (2) | H15B—C15—H15C | 109.5 |
| C8—C9—C10 | 117.5 (3) | C7—N1—C1 | 128.5 (2) |
| C8—C9—C15 | 122.5 (3) | C7—N1—H1N | 117 (2) |
| C10—C9—C15 | 120.0 (3) | C1—N1—H1N | 115 (2) |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.7 (3) | C7—C8—C9—C10 | 175.1 (3) |
| N1—C1—C2—C3 | 177.5 (2) | C13—C8—C9—C15 | 179.2 (3) |
| C1—C2—C3—C4 | 0.5 (4) | C7—C8—C9—C15 | −4.4 (4) |
| C1—C2—C3—C14 | −179.5 (3) | C8—C9—C10—C11 | −0.1 (5) |
| C2—C3—C4—C5 | −0.2 (4) | C15—C9—C10—C11 | 179.4 (4) |
| C14—C3—C4—C5 | 179.8 (3) | C9—C10—C11—C12 | 1.7 (6) |
| C3—C4—C5—C6 | 0.1 (5) | C10—C11—C12—C13 | −1.7 (7) |
| C2—C1—C6—C5 | 0.7 (4) | C11—C12—C13—C8 | 0.3 (6) |
| N1—C1—C6—C5 | −177.7 (3) | C9—C8—C13—C12 | 1.3 (5) |
| C4—C5—C6—C1 | −0.4 (5) | C7—C8—C13—C12 | −175.2 (3) |
| O1—C7—C8—C13 | 122.6 (3) | O1—C7—N1—C1 | −3.0 (4) |
| N1—C7—C8—C13 | −56.2 (3) | C8—C7—N1—C1 | 175.7 (2) |
| O1—C7—C8—C9 | −53.9 (3) | C6—C1—N1—C7 | −159.7 (2) |

| | | | |
|---|---|---|---|
| N1—C7—C8—C9 | 127.4 (2) | C2—C1—N1—C7 | 22.0 (4) |
| C13—C8—C9—C10 | −1.3 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···O1$^{i}$ | 0.84 (2) | 2.10 (2) | 2.908 (3) | 163 (3) |

Symmetry code: (i) −*y*+1, *x*, *z*−1/4.