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N-(4-Methylphenyl)benzamide

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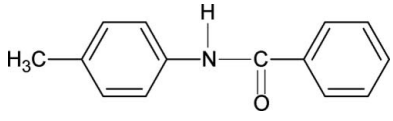
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.084; data-to-parameter ratio = 15.3.

The structure of the title compound, $C_{14}H_{13}NO$, resembles those of *N*-(2-chlorophenyl)benzamide, 2-chloro-*N*-phenylbenzamide, *N*-(2,3-dichlorophenyl)benzamide, *N*-(3,4-dichlorophenyl)benzamide and 2-chloro-*N*-(2-chlorophenyl)benzamide with similar bond parameters. The benzene and methylphenyl rings have a dihedral angle of 63.41 (5)°, while the amide group makes a dihedral angle of 20.5 (1)° with the benzene ring. The molecules are linked into chains in the *b*-axis direction by N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2003, 2007*a*,*b*,*c*); Gowda, Foro *et al.* (2007).



Experimental

Crystal data

$C_{14}H_{13}NO$
M_r = 211.25
Orthorhombic, *Pbca*
a = 9.1117 (3) Å
b = 9.8336 (2) Å
c = 26.0616 (10) Å
V = 2335.14 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.26 × 0.07 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: none
21626 measured reflections
2276 independent reflections
1060 reflections with $I > 2\sigma(I)$
R_{int} = 0.078

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.084
S = 0.82
2276 reflections
149 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 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—H1N···O1^{i}	0.826 (14)	2.117 (15)	2.9208 (14)	164.2 (15)

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997), *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2632).

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N-(4-Methylphenyl)benzamide

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S1. Comment

In the present work, the structure of *N*-(4-methylphenyl)-benzamide (N4MPBA) has been determined to explore the effect of substituents on the structure of *N*-aromatic amides (Gowda *et al.*, 2003, 2007*a*, *b*, *c*, *d*). The structure of N4MPBA (Fig. 1) resembles those of *N*-(2-chlorophenyl)-benzamide (N2CPBA) (Gowda *et al.*, 2007*a*), 2-chloro-*N*-(phenyl)-benzamide (NP2CBA) (Gowda *et al.*, 2003), *N*-(2,3-dichlorophenyl)benzamide (N23DCPBA) (Gowda *et al.*, 2007*b*), *N*-(3,4-dichlorophenyl)-benzamide (N34DCPBA)(Gowda *et al.*, 2007*c*) and 2-chloro-*N*- (2-chlorophenyl)-benzamide (N2CP2CBA) (Gowda *et al.*, 2007*d*), The bond parameters in N4MPBA are similar to those in N2CPBA, NP2CBA, N23DCPBA, N34DCPBA and N2CP2CBA. The molecules of N4MPBA are linked into chains in the direction of *b* axis through N—H···O hydrogen bonds (Table 1 and 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

H atoms bonded to C atoms were placed in geometrically calculated positions and subsequently treated as riding with C–H distances of 0.93Å for $C_{aromatic}$—H and C_{methyl}—H = 0.96 Å. The amino H atom was visible in difference map. In the refinement the N–H distance was restrained to 0.86 (5) Å. The U_{iso}(H) values were set at 1.2 U_{eq}(C,*N*) of the parent atom (1.5 for methyl).

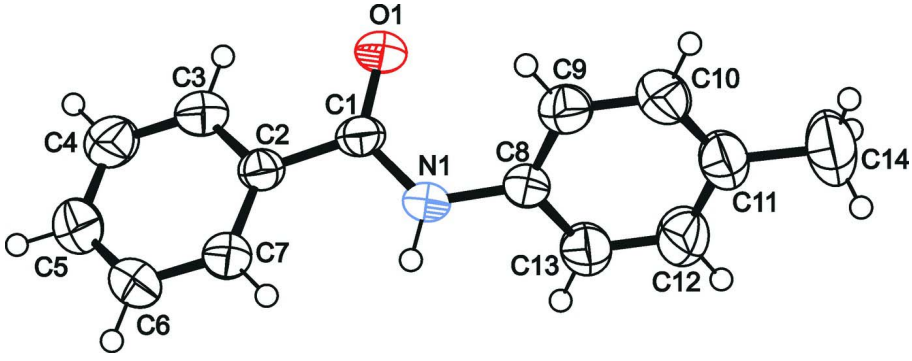

Figure 1

Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

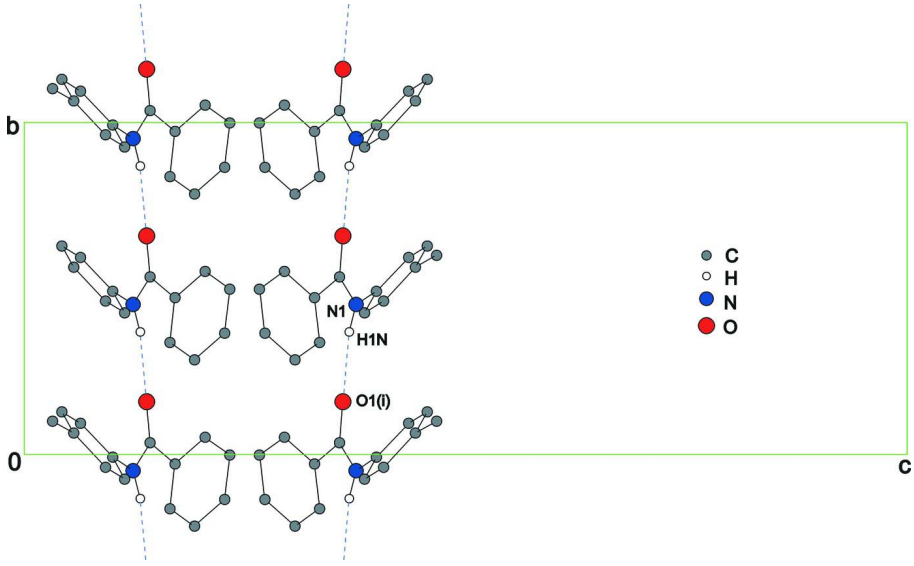

Figure 2

Partial packing diagram of the title compound showing the hydrogen bonds as dashed lines. Symmetry code (i): -*x* + 1/2, *y* - 1/2, *z*.

N-(4-Methylphenyl)benzamide

Crystal data

$C_{14}H_{13}NO$
$M_r = 211.25$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 9.1117\ (3)$ Å
$b = 9.8336\ (2)$ Å
$c = 26.0616\ (10)$ Å
$V = 2335.14\ (13)$ Å^3
$Z = 8$
$F(000) = 896$
$D_x = 1.202$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4170 reflections
$\theta = 3.1–29.4°$
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Prism, colourless
0.26 × 0.07 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Graphite monochromator
Detector resolution: 10.434 pixels mm^{-1}
ω scans with κ offsets
21626 measured reflections
2276 independent reflections
1060 reflections with $I > 2\sigma(I)$
$R_{int} = 0.078$
$\theta_{max} = 26.0°$, $\theta_{min} = 5.5°$
$h = -11\rightarrow11$
$k = -10\rightarrow12$
$l = -32\rightarrow32$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.084$
$S = 0.82$
2276 reflections
149 parameters
1 restraint
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

$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.10$ e Å^{-3}

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}
C1	0.17469 (16)	0.53524 (13)	0.35738 (6)	0.0451 (4)
C2	0.04977 (15)	0.47251 (12)	0.32925 (5)	0.0426 (4)
C3	−0.02778 (18)	0.55216 (14)	0.29516 (6)	0.0564 (4)
H3	−0.0029	0.6433	0.2912	0.068*
C4	−0.1411 (2)	0.49840 (16)	0.26710 (7)	0.0677 (5)
H4	−0.1916	0.5529	0.2439	0.081*
C5	−0.1804 (2)	0.36530 (16)	0.27305 (7)	0.0699 (5)
H5	−0.2574	0.3294	0.254	0.084*
C6	−0.10609 (19)	0.28486 (14)	0.30715 (7)	0.0637 (5)
H6	−0.1336	0.1945	0.3116	0.076*
C7	0.00930 (17)	0.33727 (13)	0.33495 (6)	0.0523 (4)
H7	0.0604	0.2818	0.3577	0.063*
C8	0.41205 (16)	0.49206 (13)	0.39957 (6)	0.0468 (4)
C9	0.4191 (2)	0.59367 (14)	0.43600 (6)	0.0568 (4)
H9	0.334	0.6383	0.4463	0.068*
C10	0.5522 (2)	0.62876 (16)	0.45704 (6)	0.0647 (5)
H10	0.5556	0.6985	0.4811	0.078*
C11	0.6797 (2)	0.56452 (16)	0.44375 (7)	0.0637 (5)
C12	0.6706 (2)	0.46213 (17)	0.40767 (7)	0.0746 (5)
H12	0.7554	0.4165	0.3978	0.089*
C13	0.53824 (19)	0.42617 (15)	0.38596 (7)	0.0664 (5)
H13	0.5348	0.3565	0.3619	0.08*
C14	0.8256 (2)	0.6010 (2)	0.46760 (8)	0.0961 (6)
H14A	0.8093	0.6467	0.4997	0.144*
H14B	0.8788	0.6599	0.4449	0.144*
H14C	0.8814	0.5197	0.4734	0.144*
N1	0.27740 (14)	0.45148 (11)	0.37649 (5)	0.0507 (4)
H1N	0.2724 (17)	0.3698 (15)	0.3692 (5)	0.061*
O1	0.18442 (12)	0.65930 (9)	0.36138 (5)	0.0701 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0446 (9)	0.0321 (7)	0.0587 (10)	0.0027 (7)	0.0071 (8)	0.0021 (7)
C2	0.0402 (9)	0.0368 (7)	0.0507 (9)	0.0018 (7)	0.0047 (8)	−0.0009 (7)
C3	0.0597 (11)	0.0416 (8)	0.0680 (10)	0.0038 (8)	−0.0024 (10)	0.0023 (8)
C4	0.0723 (13)	0.0580 (10)	0.0728 (12)	0.0102 (9)	−0.0188 (10)	−0.0002 (8)
C5	0.0637 (12)	0.0671 (11)	0.0790 (13)	0.0011 (9)	−0.0185 (11)	−0.0146 (9)
C6	0.0634 (12)	0.0464 (9)	0.0812 (12)	−0.0078 (8)	−0.0085 (11)	−0.0025 (8)
C7	0.0505 (10)	0.0421 (8)	0.0643 (11)	−0.0002 (8)	−0.0041 (9)	0.0030 (7)
C8	0.0461 (10)	0.0365 (7)	0.0577 (10)	−0.0016 (8)	−0.0048 (8)	0.0016 (7)
C9	0.0591 (12)	0.0516 (8)	0.0596 (10)	0.0054 (8)	−0.0017 (9)	−0.0043 (8)
C10	0.0702 (14)	0.0606 (10)	0.0633 (11)	−0.0037 (10)	−0.0105 (11)	−0.0100 (8)
C11	0.0572 (12)	0.0660 (11)	0.0680 (12)	−0.0118 (9)	−0.0075 (10)	0.0018 (9)
C12	0.0497 (12)	0.0822 (11)	0.0918 (13)	0.0039 (10)	0.0009 (11)	−0.0187 (11)
C13	0.0523 (12)	0.0645 (10)	0.0824 (12)	0.0044 (9)	−0.0031 (10)	−0.0238 (8)
C14	0.0670 (14)	0.1123 (14)	0.1092 (16)	−0.0196 (11)	−0.0240 (13)	−0.0088 (12)
N1	0.0502 (9)	0.0308 (5)	0.0710 (9)	0.0014 (7)	−0.0082 (7)	−0.0033 (6)
O1	0.0606 (8)	0.0331 (6)	0.1165 (9)	0.0002 (5)	−0.0177 (7)	−0.0001 (5)

Geometric parameters (Å, º)

C1—O1	1.2276 (13)	C8—C9	1.380 (2)
C1—N1	1.3425 (17)	C8—N1	1.4235 (18)
C1—C2	1.4878 (19)	C9—C10	1.375 (2)
C2—C3	1.3792 (19)	C9—H9	0.93
C2—C7	1.3880 (18)	C10—C11	1.367 (2)
C3—C4	1.371 (2)	C10—H10	0.93
C3—H3	0.93	C11—C12	1.380 (2)
C4—C5	1.366 (2)	C11—C14	1.511 (2)
C4—H4	0.93	C12—C13	1.378 (2)
C5—C6	1.369 (2)	C12—H12	0.93
C5—H5	0.93	C13—H13	0.93
C6—C7	1.377 (2)	C14—H14A	0.96
C6—H6	0.93	C14—H14B	0.96
C7—H7	0.93	C14—H14C	0.96
C8—C13	1.367 (2)	N1—H1N	0.826 (14)
O1—C1—N1	121.86 (14)	C10—C9—C8	119.79 (16)
O1—C1—C2	120.61 (13)	C10—C9—H9	120.1
N1—C1—C2	117.50 (11)	C8—C9—H9	120.1
C3—C2—C7	118.48 (13)	C11—C10—C9	122.19 (15)
C3—C2—C1	118.29 (11)	C11—C10—H10	118.9
C7—C2—C1	123.22 (13)	C9—C10—H10	118.9
C4—C3—C2	120.69 (13)	C10—C11—C12	117.29 (16)
C4—C3—H3	119.7	C10—C11—C14	122.26 (17)
C2—C3—H3	119.7	C12—C11—C14	120.44 (17)
C5—C4—C3	120.40 (15)	C13—C12—C11	121.31 (16)

C5—C4—H4	119.8	C13—C12—H12	119.3
C3—C4—H4	119.8	C11—C12—H12	119.3
C4—C5—C6	119.87 (15)	C8—C13—C12	120.52 (15)
C4—C5—H5	120.1	C8—C13—H13	119.7
C6—C5—H5	120.1	C12—C13—H13	119.7
C5—C6—C7	120.19 (14)	C11—C14—H14A	109.5
C5—C6—H6	119.9	C11—C14—H14B	109.5
C7—C6—H6	119.9	H14A—C14—H14B	109.5
C6—C7—C2	120.34 (14)	C11—C14—H14C	109.5
C6—C7—H7	119.8	H14A—C14—H14C	109.5
C2—C7—H7	119.8	H14B—C14—H14C	109.5
C13—C8—C9	118.87 (15)	C1—N1—C8	125.84 (11)
C13—C8—N1	118.86 (13)	C1—N1—H1N	118.2 (11)
C9—C8—N1	122.26 (14)	C8—N1—H1N	114.6 (11)
O1—C1—C2—C3	19.6 (2)	N1—C8—C9—C10	180.00 (13)
N1—C1—C2—C3	−158.31 (13)	C8—C9—C10—C11	−1.1 (2)
O1—C1—C2—C7	−161.61 (14)	C9—C10—C11—C12	0.4 (2)
N1—C1—C2—C7	20.5 (2)	C9—C10—C11—C14	−178.73 (15)
C7—C2—C3—C4	−0.8 (2)	C10—C11—C12—C13	0.0 (3)
C1—C2—C3—C4	178.06 (14)	C14—C11—C12—C13	179.16 (17)
C2—C3—C4—C5	0.9 (2)	C9—C8—C13—C12	−1.0 (2)
C3—C4—C5—C6	−0.1 (3)	N1—C8—C13—C12	−179.66 (14)
C4—C5—C6—C7	−0.9 (3)	C11—C12—C13—C8	0.3 (3)
C5—C6—C7—C2	1.0 (2)	O1—C1—N1—C8	−5.0 (2)
C3—C2—C7—C6	−0.2 (2)	C2—C1—N1—C8	172.86 (13)
C1—C2—C7—C6	−178.97 (14)	C13—C8—N1—C1	−134.60 (15)
C13—C8—C9—C10	1.4 (2)	C9—C8—N1—C1	46.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.83 (1)	2.12 (2)	2.9208 (14)	164 (2)

Symmetry code: (i) −*x*+1/2, *y*−1/2, *z*.